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The micro-structure of the intergalactic medium – I. The 21 cm signature from dynamical minihaloes

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ABSTRACT
A unified description is provided for the 21 cm signatures arising from minihaloes against a bright background radio source and against the cosmic microwave background (CMB), within the context of a dynamical collapsing cosmological spherical halo. The effects of gas cooling via radiative atomic and molecular processes and of star formation on setting the maximum mass of the minihaloes giving rise to a 21 cm signal are included. Models are computed both with and without molecular hydrogen formation, allowing for its possible suppression by an ambient ultraviolet radiation field. The spectral signatures and equivalent width distributions are computed for a cold dark matter cosmology. The detectability of minihaloes in absorption against bright background radio sources is discussed in the context of future measurements by a Square Kilometre Array (SKA) and the LOw Frequency ARray (LOFAR). The brightness temperature differential relative to the CMB is also computed.

Several generic scenarios are considered. For the cosmological parameter constraints from the Wilkinson Microwave Anisotropy Probe (WMAP), in the absence of any form of galactic feedback, the number of systems per unit redshift in absorption against a bright radio source at $8 < z < 10$ is $dN/dz \simeq 10$ for observed equivalent widths exceeding 0.1 kHz. For larger equivalent widths, somewhat fewer systems are predicted at increasing redshifts. The estimated numbers are independent of the presence of star formation in the haloes following molecular hydrogen formation except for rare, high equivalent width systems, which become fewer. LOFAR could plausibly detect a minihalo signal against a 30 mJy source in a 1200 h integration. SKA could detect the signal against a weaker 6 mJy source in as little as 24 h. Adding cosmological constraints from the Atacama Cosmology Telescope (ACT) suppresses the predicted number of all the absorbers by as much as an order of magnitude. In the presence of a background of ambient Ly$\alpha$ photons of sufficient intensity to couple the gas spin temperature to the kinetic temperature, as may be produced by the first star-forming objects, the number of weak absorption systems is substantially boosted, by more than two orders of magnitude, rendering the signal readily detectable. Weak absorption features arising from the cold infalling regions around the minihaloes may appear as mock emission lines relative to the suppressed continuum level. A moderate amount of heating of the intergalactic medium (IGM), however, would greatly reduce the overall number of absorption systems.

By contrast, the absorption signal of minihaloes against the CMB is distinguishable from the diffuse IGM signature only for a limited scenario of essentially no feedback and moderate redshifts, $z < 19$. The strength of the signal is dominated by the more massive minihaloes, and so is sensitive to a cut-off in the upper minihalo mass range imposed by any star formation and its consequences. Once the first star-forming systems provide feedback in the form of Ly$\alpha$ photons, the diffuse IGM signal will quickly dominate the signal from minihaloes because of the small total fraction of IGM mass in the minihalo cores.

Key words: molecular processes – galaxies: formation – intergalactic medium – cosmology: theory – dark ages, reionization, first stars – radio lines: general.
1 INTRODUCTION

A principal science goal of the Square Kilometre Array (SKA) is the detection of neutral hydrogen in the intergalactic medium (IGM) following the recombination epoch and prior to the Epoch of Reionization (EoR), performing 3D tomography of the filamentary large-scale structure of the Universe as revealed by neutral hydrogen at the end of the Dark Ages when the first sources of light emerge in the Universe after the big bang (Hogan & Rees 1979; Scott & Rees 1990; Madau, Meiksin & Rees 1997). Even before SKA is built, the absorption of a still largely neutral IGM may be detectable against radio-loud galaxies or quasars by SKA pathfinders like the LOFAR (LOFAR) and the Long Wavelength Array (LWA), both already underway, and the Murchison Widefield Array (MWA), a SKA precursor facility soon to start.

Extracting the EoR signal from the radio data is a major undertaking requiring modelling of both the expected 21 cm signature and the effects of contaminating sources which will swamp the underlying cosmological signal (Hogan & Rees 1979; Shaver et al. 1999; Morales, Bowman & Hewitt 2006; Jelić et al. 2008). The extraction of the EoR signature is further complicated by uncertainties in the signature itself arising from the unknown manner in which the Universe was reionized and from the structure of the IGM. The 21 cm signals will be highly patchy, as the cold hydrogen atoms will closely trace the filamentary structure of the dark matter in the Universe on large scales and the non-linear fluctuations in the dark matter on the very small. If a bright background radio source is present, the intervening neutral hydrogen in the IGM will produce an absorption signature against it, with a strength depending on the temperature of the IGM and how efficiently the spin temperature is coupled to it (Field 1959a). The IGM will also produce a fluctuating signal against the cosmic microwave background (CMB) (Hogan & Rees 1979; Scott & Rees 1990; Tozzi et al. 2000), either in absorption or in emission depending on the gas kinetic temperature compared with the CMB temperature. Only on scales small compared with the Jeans length of the gas will the IGM produce a smooth signal. The neutral hydrogen thus provides a unique means of measuring the power spectrum of dark matter over a wide range of length-scales spanning six decades at the as yet unprobed epochs between the Recombination Era and the emergence of the first galaxies.

Perhaps the best near-term prospect for detecting a still neutral IGM is in absorption against a bright background radio source. Collapsed minihaloes will produce a 21-cm forest of absorption features in the radio spectrum of such a source (Carilli, Gnedin & Owen 2002; Furlanetto & Loeb 2004). This claim has been disputed by Oh & Mack (2003), who objected that, because of the overwhelming amount of mass in the diffuse IGM compared with minihaloes, except very early on before there is any feedback from galaxies, the diffuse component will dominate. It has been argued biased boosts the brightness temperature fluctuations significantly only on scales too small to be measured with currently planned radio facilities (Furlanetto & Oh 2006). Numerical simulations have tended to support these expectations (Kuhlen, Madau & Montgomery 2006; Yue et al. 2009). Using an extension of the Press–Schechter formalism, Furlanetto & Loeb (2004) suggested that even without galactic feedback, the 21 cm signal from the shocked diffuse IGM would exceed that due to the minihaloes. High spatial resolution numerical simulations by Kuhlen et al. (2006) appear to confirm this claim, although the opposing view has again been defended by Shapiro et al. (2006).

Estimates of the strength of the 21 cm signature from minihaloes are made uncertain by several poorly known factors. The number density of the haloes is notoriously difficult to quantify, especially since the minihaloes arise on scales for which the dark matter power spectrum is approaching the ‘flicker noise’ small-scale limit, for which structures on all scales collapse and virialize simultaneously. Numerical simulations are currently not of much help for estimating the distribution of dark matter haloes or their internal structure on all the relevant scales, as it is not yet possible to capture the power over the full dynamic range required.

Another major outstanding uncertainty is the effect of the first generation of stars on subsequent star formation. Early models suggested Lyman–Werner photons from the first stars will dissociate molecular hydrogen in the surrounding gas and inhibit star formation in haloes with temperatures below 10^4 K, when atomic cooling dominates (Haiman, Rees & Loeb 1997a, b). Subsequent analyses have shown the picture is much more complicated. Self-shielding will limit the radiative transport of the Lyman–Werner photons, although by an amount that generally depends on internal flows (Glover & Brand 2001). Whilst hot stars will photoionize their surroundings, partial ionization may enhance the rate of molecular hydrogen formation, as would sources of X-rays, negating the dissociating effects of the UV radiation from early sources (Haiman, Abel & Rees 2000). Within relic H I regions, molecular hydrogen reforms as the gas recombines, re-enabling star formation. The injection of dust would provide still an additional mechanism for molecular hydrogen formation. The injection of metals from

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1 www.skatelescope.org
2 www.lofar.org
3 wa.phys.unm.edu
4 www.mwatelescope.org

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supernovae would accelerate cooling. The feedback from star formation on subsequent generations of stars has been considered widely in the literature (e.g. Couchman & Rees 1986; Mac Low & Shull 1986; Dekel & Rees 1987; Ostriker & Gnedin 1996; Haiman, Rees & Loeb 1997a; Omukai & Nishi 1999; Glover & Brand 2001; Machacek, Bryan & Abel 2001; O’Shea et al. 2005; Yoshida et al. 2007; Wise & Abel 2007; Whalen et al. 2008; Mesinger, Bryan & Haiman 2009; Whalen, Hueckstaedt & McConkie 2010; Gnedin 2010).

Even if the first stars produce local pockets of Lyman–Werner photons, it is unknown whether or not a metagalactic radiation field ever develops that is sufficiently intense to dissociate molecular hydrogen in minihaloes everywhere, or the epoch at which such a field develops if it does. Indeed, one of the primary goals of the search for an intergalactic 21 cm signature is to establish the epoch of star formation and quantify its large-scale distribution. To allow for the possibility that the first generation of stars either only partially or completely inhibits subsequent molecular hydrogen formation, two sets of models are computed, one allowing for molecular hydrogen formation and a second with molecular hydrogen formation suppressed.

Early massive stars may also produce X-rays, particularly after they explode as supernovae and heat their surroundings to high temperatures. Other possible sources of X-rays include early active galactic nuclei (AGN) and collapsed structures shock-heated to X-ray temperatures (Madau et al. 1997; Tozzi et al. 2000; Carilli et al. 2002; Furlanetto & Loeb 2004; Kuhlen et al. 2006). The amount of heating is unknown. Substantial heating would reduce the collapse fraction of the gas into minihaloes, weakening their 21 cm signature. But even a small amount too little to much affect the dynamics of the gas will reduce the absorption signal against a bright background radio source, and could change an absorption signal against the CMB into emission if the IGM temperature increases above that of the CMB.

The primary purpose of this paper is to address the effect of some of these assumptions and uncertainties on the expected 21 cm signatures from minihaloes. Only single-point statistics are addressed, relating to the absorption signature of minihaloes against a bright background radio source, or the differential brightness temperature against the CMB based on comparing the signal along the line of sight through a neutral patch with that through an ionized patch. Cross-correlation measurements, particularly as have been considered in the context of measurements against the CMB, require estimates of the halo bias factors and spatial correlations between the minihaloes. Correlated fluctuations arising from the diffuse IGM are also expected to be a major contributor. These topics are beyond the scope of this paper.

In previous models of the 21 cm signature from minihaloes, the minihaloes have generally been assumed to be isothermal and in hydrostatic equilibrium. It was recognized in the context of the minihalo model for Lyα forest absorption systems (Ikeuchi 1986; Rees 1986) that the systems will in general be formed in dynamically collapsing (Bond, Szalay & Silk 1988) and non-isothermal (Meiksin 1994) dark matter haloes. Allowing for the dynamics introduces modifications to the thermal structure and pressure support of the gas in the minihaloes, which in turn modify the cross-sections for their detection.

The haloes are evolved as spherical density perturbations. Treating the haloes as arising from isolated perturbations is itself an approximation, as in bottom-up scenarios like cold dark matter dominated cosmologies, structures are created from the merger of smaller systems. In this sense, the perturbations are more representative of an evolving patch of smaller haloes which merge into the final collapsed structure. In the early stages of evolution, even this is not a good approximation as the overdense patches are typically triaxial (Bardeen et al. 1986, hereafter BBKS), and embedded in a large-scale filamentary network, the cosmic web (Bond, Kofman & Pogosyan 1996). Simulations suggest, however, that spheroidal structures do form; the spherical minihalo model provides a useful description of the higher column density systems within the Lyα forest (Rauch 1998; Meiksin 2009).

The collapsing spherical halo approximation has the advantage over the static isothermal halo approximation of allowing the density and temperature profiles to arise naturally during the collapse of the halo. The modelling of an evolving system also reveals some of the dynamical effects which may play an important role in the cooling of the gas and in determining the minimum halo mass at which star formation sets in. It is argued that only a small number of stars need form before the remaining gas in the minihalo will be expelled through mechanical feedback due to photo-evaporative winds and supernovae. The rate of star formation is modelled to provide an estimate for the upper limiting minihalo mass at any given collapse epoch. (More massive systems than minihaloes become increasingly complex, such as forming galaxy haloes and their associated discs, and are not considered here.)

Only the 21 cm signal from fully collapsed haloes, along with their surrounding infall regions, is considered in this paper. Sufficiently dense gas within the filaments will also contribute to the 21 cm signal. The treatment of such moderate overdense structures is less straightforward to model and so is deferred to a later work, although comparison is made with the total signal that could potentially arise from a diffuse homogeneous component. Ultimately a very high resolution fully 3D combined dark matter and hydrodynamics simulation would be required for a precise prediction of the expected 21 cm signatures.

A second purpose of this paper is to provide a semi-analytic framework that incorporates the dynamical effects to estimate the 21 cm signals from minihaloes. Numerical simulations are still unable to resolve the full range of scales required to estimate the 21 cm signature without some semi-analytic modelling, and even if they were able to do so, they are very costly to run. Alternative halo mass distributions may be readily explored within the semi-analytic framework. The 21 cm signatures produced by minihaloes probe a part of the cosmological dark matter power spectrum that has never been measured at high redshifts, down to scales on the order of a comoving kiloparsec, or a millionth of the cosmological horizon. The effect of different cosmological scenarios, such as alterations to the small-scale power spectrum, may be readily examined within the framework. It is demonstrated below that the minihalo 21 cm signature may in fact provide a useful means for distinguishing between rival predictions for the amount of power on small scales.

Unless stated otherwise, the present-day values of the cosmological parameters assumed are Ω_M = 0.27, Ω_Λ = 0.73, Ω_b = 0.0456, h = 0.70, σ8h^−1 = 0.81 and n = 0.96 for the total mass, vacuum energy and baryon density parameters, the Hubble constant (h = H_0/100 km s^−1 Mpc^−1), the linear density fluctuation amplitude on a scale of 8h^−1 Mpc and the spectral index, respectively, consistent with CMB measurements by the Wilkinson Microwave Anisotropy Probe (WMAP) (Komatsu et al. 2009, 2011).

This paper is organized as follows. The next section presents basic relations for evaluating the 21 cm signatures from minihaloes, and applies these to the simple model of tophat minihaloes with uniform densities that provides a fiducial for comparing the more complete dynamical models against. Section 3 describes the
dynamical minihalo model and presents the 21 cm signatures arising from individual haloes. In Section 4, the individual minihalo signatures are combined to model the expected statistical signals from the haloes. The statistical signals are discussed in various cosmological scenarios in Section 5. A summary of the principal findings and conclusions is provided in Section 6. Semi-analytic estimates for the post-collapse temperatures of minihaloes, their abundances, and the computation of molecular hydrogen formation are discussed in separate Appendices.

2 21CM SIGNATURE OF TOPHAT MINIHALOES

2.1 Spectral characteristics of tophat minihaloes

The diffuse component of the IGM at redshift \( z \) will produce a relative differential brightness temperature against a background source of observed antenna temperature \( T_B(0) \) of

\[
\frac{\delta T_B(0)}{T_B(0)} = \left[ \frac{T_S}{T_B(0)(1+z)} - 1 \right] [1 - \exp(-\tau_d)]
\]

\[
\approx -\tau_d \left[ 1 - \frac{T_S}{T_B(0)(1+z)} \right]
\]

where the 21 cm optical depth of the IGM with mean hydrogen density \( n_H(z) \), neutral fraction \( x_H(z) \) and spin temperature \( T_S(z) \) is given by

\[
\tau_d = \frac{3}{32\pi} x_H(1+\delta(z))n_H(z)^{1/3} \frac{A_{10} T_S}{H(z)} \frac{1}{T_B(0)} \frac{1}{[\text{d}u(1)/\text{d}l]/H(z)}
\]

\[
\approx 0.0046[1 + \delta(z)] \left( \frac{T_S(z)}{T_B(0)} \right) \Omega_m^{-1/2}(1+z)^{3/2}
\]

\[
\times \left[ 1 + \frac{1 - \Omega_m}{\Omega_m (1+z)^{3/2}} \right]^{-1/2} \frac{1}{[\text{d}u(1)/\text{d}l]/H(z)}
\]

(1)

with \( T_B = T_B(0)(1+z) \), and where \( T_S = h\nu/\lambda_b \), \( \lambda_b \approx 21.1 \) cm, \( \nu_{10} = c\lambda_{10}/\lambda_b \) is the Boltzmann constant, \( A_{10} \approx 2.85 \times 10^{-15} \) s⁻¹ is the spontaneous transition rate of the 21 cm hyperfine transition, and allowing for linear density fluctuations \( \delta(z) \) (Field 1959a; Scott & Rees 1990; Madau et al. 1997; Meiksin 2009). The spin temperature is given by

\[
T_S = T_{CMB}(z) + y_a T_a + y_c T_c
\]

\[
= T_{CMB}(z) + \frac{y_a T_a + y_c T_c}{1 + y_a + y_c}
\]

(3)

(Feild 1958), where \( y_a = (P_{10}/A_{10})(T_a/T_B) \) for a de-excitation rate \( P_{10} \) of the hyperfine triplet state by Ly\( \alpha \) photon scattering at the rate \( P_{10} = (27/4)P_{10} \), \( y_a \) is the colour temperature of the radiation field, \( y_c = (C_{10}/A_{10})(T_a/T_B) \) for a collisional de-excitation rate \( C_{10} \) of the hyperfine triplet state, where \( k_{1-0} \) is the de-excitation rate coefficient, \( T_k \) is the kinetic temperature of the gas and \( T_{CMB}(z) \) is the CMB temperature at redshift \( z \). The colour temperature relaxes rapidly to the gas kinetic temperature after 10⁴ scattering times (Field 1959b; Meiksin 2006), so that \( T_a = T_k \) is assumed. For a Ly\( \alpha \) scattering rate \( P_{10} \) matching the collisional rate \( P_{10} = (27/4)A_{10} T_{CMB}(z)/T \), the radiation field effectively couples the spin temperature to the kinetic temperature of the gas (Madau et al. 1997). The collisional de-excitation rate coefficient \( \kappa_{1-0} \) is interpolated from the tables of Zylgeman (2005) for \( T \leq 300 \) K and Allison & Dalgarno (1969) for \( T > 300 \) K, using 4/3 the latter’s tabulated values as advocated by Zylgeman (2005). The optical depth will typically be much smaller than unity. The signal will be in either emission or absorption against the background source, depending on the larger of \( T_S \) and \( T_B(0)(1+z) \).

Superposed on any signature from the diffuse IGM in the spectrum of a background radio source will be narrow features produced by intervening minihaloes. These again will be in either emission or absorption, depending on the brightness temperature of the source. Whilst the collapsed haloes will develop a steep internal density profile, it is useful to formulate the contribution of the minihaloes in the simplified scenario of collapsing isothermal spherical tophats. Although a simplification, it provides a straightforward fiducial model that incorporates most of the essential physics against which more sophisticated models may be compared. In particular, in the limit of negligible dissipation, it provides the expected scaling relations of the mean equivalent width on the cosmological parameters and the redshift of collapse.

The differential brightness temperature produced by intervening gas against a background source of brightness temperature \( T_B(v) \) is given by

\[
\delta T_B(v) = \int \frac{\text{d}l}{\text{d}t} T_B(l) \frac{\text{d}x}{\text{d}t} e^{-\tau_v(l)} - T_B(v)(1 - e^{-\tau_v(v)}),
\]

where

\[
\tau_v(l) = \frac{3}{8\pi} A_{10} \lambda_{10}^3 \int \frac{\text{d}l}{\text{d}t} \frac{1}{4} x_H(l) n_H(l) \phi_l \frac{T_{CMB}(l)}{T_B(l)}
\]

(5)

is the optical depth from the source up to a distance \( l \) through the intervening gas of total hydrogen density \( n_H(l) \), neutral fraction \( x_H(l) \) and spin temperature \( T_S(l) \). The factor 1/4 accounts for the occupation fraction of the lower hyperfine level of the hydrogen. The factor \( T_S(l)/T_B \) accounts for stimulated emission of the 21 cm line. The absorption line profile is described by \( \phi_l = \phi_\infty \Delta \nu_p \), where \( \phi_\infty = \pi^{-1/2} \exp\left\{-[v - v_{10}(1 - v(l)/c)]^2/(\Delta \nu_p)^2\right\} \) is the dimensionless Doppler profile with Doppler width \( \Delta \nu_p = (b c) \nu_p \) and Doppler parameter \( b = (2 k_B T_{gas})^{1/2} \), where \( T \) is the gas temperature. Estimates for the gas temperature in collapsed minihaloes are presented in Appendix A. The Doppler shifting of the line centre frequency by the bulk motion of the gas with flow velocity \( v(l) \) along the line of sight has been allowed for in the optical depth.

The observed equivalent width through an individual tophat halo at a projected comoving separation \( b_\perp \) from the centre is given by

\[
w_{\text{obs}}(b_\perp) = \pm (1+z)^{-1} \int \text{d}v \frac{\delta T_B(v)}{T_B}
\]

\[
= \pm (1+z)^{-1} \left[ \frac{T_S}{T_{CMB}(z)} - 1 \right] \int \text{d}v (1 - e^{-\tau_v(b_\perp)\nu})
\]

(6)

where the redshift factor converts the rest-frame equivalent width to the observed frame, and the sign convention is chosen so that the equivalent width is made positive whether corresponding to emission or absorption. Here, \( \tau_v = \tau_v c \pi^{-1/2} \Delta \nu_p g_\nu \). Assuming the gas is isothermal and in hydrostatic equilibrium, the line centre optical depth \( \tau_0 \) for a spherical tophat collapsed at redshift \( z \) is given by

\[
\tau_0 = \frac{3}{8\pi} A_{10} \lambda_{10}^3 f_c^{-2} x_H(z)^2 \frac{T_S}{4b} \left[ 1 - \left( \frac{b_\perp}{f_c r_0} \right)^2 \right] T_{CMB}(z)
\]

(7)

where the halo virializes at radius \( r_v = f_c r_0(1 + z) \) with \( f_c = (18\pi^2)^{-1/3} \). The factor \( f_c^{-2} \) accounts for the increased column density through the collapsed halo.

Typically \( \tau_0 \ll 1 \), in which case the observed equivalent width of a halo of mass \( M \) collapsed at redshift \( z \) may be expressed as

\[
w_{\text{obs}}(b_\perp) = w_{\text{obs}}(0) \left( 1 - \frac{b_\perp}{f_c r_0} \right)^{1/2}
\]

(8)
where

\[ w_{\text{obs}}^{\text{abs}}(0) = \pm \frac{3}{32\pi} A_{\nu} \lambda_0^2 \frac{f_{\nu}}{f_{\nu}} x_{\text{H}} r_{\text{H}}(0) x_{\text{H}}^2(M) \]

\times \left( 1 + z^3 \right) \int \frac{dV_{\text{obs}}^{\text{abs}}}{dz} \frac{\partial^2 N}{\partial N_{\text{obs}}^{\text{abs}} \partial z} w_{\text{obs}}^{\text{abs}},

(9)

It will be shown below that for either absorption against a bright radio source or absorption or emission against the CMB, the observed equivalent width is independent of the redshift of the minihalo, depending only on its mass.

The combined absorption by the minihaloes will reduce the antenna temperature by \( \exp(-\tau_i) \), so that \( T_B(0) = -T_B(0)(1 - e^{-\tau_i}) \), where

\[ \tau_i = \frac{1}{v_{10}} \left( 1 + z_c^2 \right) \int \frac{dV_{\text{obs}}^{\text{abs}}}{dz} \frac{\partial^2 N}{\partial N_{\text{obs}}^{\text{abs}} \partial z} w_{\text{obs}}^{\text{abs}}, \]

(10)

where \( \partial^2 N/\partial V_{\text{obs}}^{\text{abs}} \partial z \) is the number of features of observed equivalent width \( w_{\text{obs}}^{\text{abs}} \) per unit redshift (Meiksin 2009). Values with either \( \tau_i > 0 \) or \( \tau_i < 0 \) are possible, corresponding to absorption or emission, respectively, against the radio background.

The equivalent width distribution may be computed as \( \partial^2 N/\partial V_{\text{obs}}^{\text{abs}} \partial z = (1 + z_c^2) \int dM dN \frac{\sigma_{\text{max}}^{\text{abs}}(M)}{\partial z} \), where \( dN(>w_{\text{obs}})/dz \) is the number of absorbers per unit redshift with observed equivalent widths exceeding \( w_{\text{obs}}^{\text{abs}} \). This is given by

\[ \frac{dN(>w_{\text{obs}})}{dz} = \frac{(1 + z_c^2)}{v_{10}} \frac{dL}{dz} \int dM \frac{dn}{dM} \frac{\sigma_{\text{max}}^{\text{abs}}(M)}{\partial z}, \]

(11)

where \( dL/dz = (cH(z)(1 + z)^{-1} \) is the differential proper length per redshift, \( dn/dM \) is the number of collapsed haloes of mass \( M \) per unit comoving volume and \( \sigma_{\text{max}}^{\text{abs}}(M) = \pi [b_{\perp} r_{\text{max}}(M)]^2 \) is the comoving cross-section corresponding to the maximum comoving impact parameter \( b_{\perp} r_{\text{max}}(M) \) through the halo within which the equivalent width exceeds \( w_{\text{obs}}^{\text{abs}} \). From equation (8), it is given by

\[ b_{\perp} r_{\text{max}} = f_{\nu_0} \left\{ 1 - \left[ \frac{w_{\text{obs}}^{\text{abs}}}{w_{\text{obs}}^{\text{abs}}(0)} \right]^2 \right\}^{1/2} \] .

(12)

The last form expresses the number density per unit redshift more generally in terms of the comoving mean free path \( \lambda_{\text{mean}}(w_{\text{obs}}^{\text{abs}}) = 1/(dn/dlog M) \sigma_{\text{max}}^{\text{abs}}(M) \), where \( \sigma_{\text{max}}^{\text{abs}}(M) \) is the cross-section through a halo of mass \( M \) giving rise to an absorption feature with observed equivalent width exceeding \( w_{\text{obs}}^{\text{abs}} \).

It follows from equation (10) that the cumulative optical depth from the ensemble of minihaloes may be expressed, after an integration by parts, as

\[ \tau_i = \frac{1}{v_{10}} \left( 1 + z_c^2 \right) \int \frac{dV_{\text{obs}}^{\text{abs}}}{dz} \frac{\partial^2 N}{\partial N_{\text{obs}}^{\text{abs}} \partial z} (>w_{\text{obs}}^{\text{abs}}) \]

\[ = \frac{1}{v_{10}} \left( 1 + z_c^2 \right) \int \frac{dL}{dz} \int_{M_{\text{min}}}^{M_{\text{max}}} dM \frac{dn}{dM} \frac{\sigma_{\text{mean}}^{\text{abs}}(M)}{\partial z} \]

\[ = \frac{1}{v_{10}} \left( 1 + z_c^2 \right) \int \frac{dL}{dz} \int_{M_{\text{min}}}^{M_{\text{max}}} dM \frac{dn}{dM} \sigma_{\text{mean}}^{\text{abs}}(M) \Sigma_w, \]

(13)

where the last form is general, with \( \Sigma_w = \sigma_b(w_{\text{obs}}^{\text{abs}}) \) the equivalent width weighted cross-section, where \( w_{\text{obs}}^{\text{abs}} \) is the mean observed equivalent width face-averaged over a comoving halo cross-section \( \sigma_b \). More generally,

\[ \Sigma_w^{\text{abs}} \left( b_{\perp}^{\text{max}} \right) = 2\pi \int_0^{b_{\perp}^{\text{max}}} db_{\perp} b_{\perp} w_{\text{obs}}^{\text{abs}}(b_{\perp}). \]

(14)

This may be compared with the optical depth through the diffuse component of the IGM. The spin temperature will quickly come to the CMB temperature, in which case the optical depth of the diffuse component would be \( \tau_i \approx 0.011 \) at \( z = 10 \). In the presence of either a sufficient collision rate with hydrogen atoms and electrons, or a sufficiently intense Ly α scattering rate, the spin temperature of the hydrogen will be coupled to the kinetic temperature of the gas. The resulting optical depth of the diffuse component would then increase to \( \tau_i \approx 0.13 \). In the presence of heating, the optical depth would be reduced inversely with increasing gas temperature.

Experiments designed to measure an IGM signal against the CMB compare the signal from a neutral patch of the IGM with that towards an ionized patch, through which the CMB signal will be negligibly attenuated. For a spin temperature coupled to the gas kinetic temperature throughout the IGM, the corresponding differential brightness temperature compared with the CMB would be \( T_B - T_{\text{CMB}} \approx -330 \text{ mK} \) at \( z = 10 \). If the IGM were heated to a temperature much higher than the CMB temperature, the differential brightness temperature against the CMB, however, would convert to emission, saturating at a value of 29 mK.

The minihalo signal against the CMB may be detectable when the amount of galactic feedback is too little to decouple the spin temperature of the diffuse IGM component from that of the CMB. Since the telescope beam probing the neutral patch will encompass a large number of minihaloes, the collective optical depth of an ensemble of minihaloes determines the strength of the minihalo signal. The expression for the optical depth takes on a particularly simple form in the approximation that the systems are optically thin. If \( \Gamma(M) \) denotes the hydrogen mass fraction of a halo of total mass \( M \), then using equation (9), the optical depth may be re-expressed as

\[ \tau_i = 3 \frac{3}{32\pi} A_{\nu} \lambda_0^2 \frac{f_{\nu}}{f_{\nu}} x_{\text{H}} r_{\text{H}}(0) \frac{T_s}{T_{\text{CMB}}(z)} \]

\[ \times \frac{1}{m_H} \int_{M_{\text{min}}}^{M_{\text{max}}} dM \frac{dn}{dM} \gamma(M) \eta_{\text{CMB}}(M), \]

(15)

where

\[ \eta_{\text{CMB}} = x_{\text{H}} \left[ 1 - T_{\text{CMB}}(z) \right] \]

\[ = \frac{\rho_{\text{H}}}{\rho_{\text{crit}}} \left[ 1 - T_{\text{CMB}}(z) \right] + \chi_H \left[ T_{\text{CMB}}(z) - 1 \right] \]

\[ + \frac{\rho_{\text{H}}}{\rho_{\text{crit}}} \chi_H T_{\text{CMB}}(z). \]

(16)

is the 21 cm efficiency for absorption [\( T_s < T_{\text{CMB}}(z) \)] or emission [\( T_s > T_{\text{CMB}}(z) \)] against the CMB (Madau et al. 1997). The last form uses equation (3). Comparison with equation (2) shows the optical depth takes on the same form as for the diffuse IGM with \( T_s(z) \) replaced by \( T_{\text{CMB}}(z) \) and \( \eta_{\text{H}}(z) \) by \( \eta_{\text{H}}(z)/(f_{\text{H}}) \), where \( (f_{\text{H}}) = [m_H \eta_{\text{H}}(0)]^{-1} \int dM(dn/dM)\gamma(M)M \eta_{\text{CMB}}(M) \). The optical depth is thus proportional to the mean hydrogen mass fraction of the IGM in haloes, weighted by the 21 cm efficiency of the haloes. The resulting observed temperature differential compared with the CMB is \( \delta T_B(0) = -\tau_i T_{\text{CMB}}(0) \).

2.2 21 cm signature against a bright radio source

The diffuse IGM will produce an absorption signature against a bright background radio source such as a quasar or radio galaxy. For a mean neutral hydrogen density given by the cosmic mean hydrogen density, and for a hyperfine structure coupled strongly to the CMB, so that \( T_s = T_{\text{CMB}}(z) \), the optical depth of the diffuse...
component is \( \tau_d \approx 0.011(1 + z)/11^{1/2} \). The absorption will appear as a step shortwards of the observed wavelength of the 21 cm line.

Superposed on the step will be deeper absorption features arising from overdense structures, the 21 cm forest. The equivalent width of a minihalo with line centre optical \( \tau_d(b_{\perp}) \) a projected distance \( b_{\perp} \) from the centre is

\[
\frac{w^\text{obs}_{\nu}}{\nu} = (1 + z)^{-1} \frac{2h}{c} \nu_0 F(\tau_d(b_{\perp})),
\]

where \( F(\tau_d) \) is a function of the line centre optical depth. For a spin temperature coupled to the post-shock temperature of the halo, using equation (A4) from Appendix A in equation (7) gives for the line centre optical depth through the core \( (b_{\perp} = 0) \)

\[
\tau_0(0) \approx 0.00275(1 + z)^{1/2} \left( \frac{M}{10^6 \, M_\odot} \right)^{-2/3}.
\]

Only the lowest mass haloes at high redshift will have \( \tau_0(0) > 0.1 \), so that the linear curve-of-growth approximation \( F(\tau_d) \approx (\pi/2)^{1/2} \tau_0 \) may generally be made.

The corresponding equivalent width may then be re-expressed as

\[
w^\text{obs}_{\nu}(0) = \frac{1}{6\pi} \left( \frac{3}{2\pi^2} \right)^{1/3} A_{10}^2 \left( \frac{\lambda_{10}}{\nu_0} \right)^2 \tilde{n}_H(0) \\
\times \left[ \frac{3\nu_0 T_\perp}{4\pi G \Omega_m \rho_{\text{crit}}(0) \tilde{n}_H} \right]^{2/3} \left( \frac{k_B T_\perp}{GM \tilde{n}_H} \right)^{1/3} \\
\approx 0.2933 \frac{\Omega_m h^2}{(\Omega_m h^2)^{1/3}} \left( \frac{M}{10^6 \, M_\odot} \right)^{-1/3} \text{kHz} \\
\approx 0.0252 \left( \frac{M}{10^6 \, M_\odot} \right)^{-1/3} \text{kHz}.
\]

It follows that the observed equivalent width is independent of the collapse redshift \( z_c \). The strongest absorption lines arise from the lowest mass haloes because of their lower temperatures. From the dependence of \( \tau_0 \) and \( w^\text{obs}_{\nu}(0) \) on \( M \), and noting from Fig. B1 that \( M^2 \, d\nu/dM \rightarrow \) constant for low-mass haloes, it follows that the absorption signal varies like \( \tau_\perp \sim M^{-2/3} \), so that it is the lowest mass haloes \( M_{\text{min}} \), those just sufficiently massive for shocks to form when they collapse, that dominate the overall signal.

The characteristic observed line width of the features is

\[
\Delta v^\text{obs}_0 \approx 5.17(1 + z_c)^{-1/2} \left( \frac{M}{10^6 \, M_\odot} \right)^{1/3} \text{kHz}.
\]

Such features would be well resolvable by an instrument with channels on the order of 1 kHz wide.

### 2.3 21 cm signature against the CMB

In addition to an absorption signature against a bright background radio source, minihaloes will produce absorption or emission against the CMB as well. The measured antenna temperature through a halo will be \( T_\perp(0) = T_{\text{CMB}(0)} \exp(-\tau_\perp) \), where \( \tau_\perp \) is again given by equation (13), where now \( T_{\text{CMB}(z)} = T_{\text{CMB}(0)}(1 + z) \) is used for \( T_\perp(z) \) in equation (9), to give

\[
w^\text{obs}_{\nu}(0) = \frac{3}{32\pi} A_{10}^2 \frac{A_{10}^2}{\nu_0} \tilde{n}_H(0) 2r_0(M) \frac{T_\perp}{T_{\text{CMB}(0)}},
\]

In principle, systems in absorption against the CMB would produce a 21 cm forest. From equation (A4) for the post-shock temperature of a halo, however, it follows that requiring \( T_{\perp} < T_{\text{CMB}(z)} \) restricts the range of halo masses in absorption to \( M \lesssim 7300 \, M_\odot \).

This is comparable to the Jeans mass, so that the signal would be very weak.

Similarly, the haloes could produce discrete emission lines against the CMB. In the limit \( T_S \gg T_{\text{CMB}(z)} \), equation (21) becomes

\[
\frac{w^\text{obs}_{\nu}(0)}{\nu} \approx 15.07 \frac{\Omega_6 h^2}{(\Omega_m h^2)^{1/3}} \left( \frac{M}{10^6 \, M_\odot} \right)^{1/3} \text{kHz} \\
\approx 0.665 \left( \frac{M}{10^6 \, M_\odot} \right)^{1/3} \text{kHz},
\]

independent of the redshift of the halo. The detection of an individual emission line in a narrow frequency channel against a signal as weak as the CMB, however, is unlikely for the foreseeable future. More viable is the average signal from an ensemble of haloes, integrated over several channels. The observed frame equivalent width weighted comoving cross-section of the haloes is given by

\[
\Sigma^\text{obs}_w \approx 135.5 \frac{\Omega_6}{\Omega_m} \left( \frac{M}{10^6 \, M_\odot} \right) \text{kHz-kpc}^2 \\
\approx 22.6 \left( \frac{M}{10^6 \, M_\odot} \right) \text{kHz-kpc}^2.
\]

In the limit \( T_S \gg T_{\text{CMB}(z)} \) and using the Press–Schechter form for the halo mass function (Press & Schechter 1974), the optical depth equation (15) may be cast in the suggestive form

\[
\tau_\perp \approx - \frac{3}{32\pi} A_{10}^2 \frac{A_{10}^2}{\nu_0} \tilde{n}_H(0) \frac{T_\perp}{T_{\text{CMB}(z)}} \\
\times \left[ \text{erf}(t_{\text{max}}) - \text{erf}(t_{\text{min}}) \right],
\]

where \( \text{erf}(t) \) is the mass fraction of the Universe in minihaloes. The signal from minihaloes is thus a small fraction of the available signal from the CMB. At redshifts \( z < 20 \), when collisional decoupling from the CMB is weak within the diffuse IGM, minihaloes may dominate the signal until Lyman resonance line radiation becomes available to sufficiently decouple the spin state of the hydrogen atoms in the diffuse IGM from the CMB. The signal from the diffuse IGM, however, will dominate over that of the minihaloes once the mass-averaged 21 cm efficiency of the diffuse component exceeds the mass fraction of the Universe in minihaloes.

As shown by the expressions above for the number of absorption features along a line of sight and their effective optical depth, the ensemble statistics of the 21 cm features depend on the number density of minihaloes. The fitting formula of Reed et al. (2007) is adopted throughout the remainder of this paper. This choice is justified in Appendix B.

### 3 THE DYNAMICAL MINIHALO MODEL

#### 3.1 Model parameterization

Spherical minihalo models for intergalactic gas clouds with the gas confined by dark matter haloes were introduced by Ikeuchi (1986) and Rees (1986), with the lower mass end limited by that required to bind photoionized gas. Recognizing that cosmological haloes are in general dynamical, with the gas either collapsing or
expanding, Bond et al. (1988) extended the models by building the haloes from growing spherical cosmological density perturbations. Since the haloes form from the merger of smaller haloes, there is some freedom in the choice of the initial linear gas density profile. Whilst a tophat perturbation is simplest, Bond et al. (1988) chose a Gaussian profile as it was found to represent the final virialized halo density profile. In this paper, a tophat initial density profile is adopted for its simplicity, since the gas density will respond to the gravitational potential of the dark matter and gas combined, which is not very sensitive to the underlying density profile of the dark matter.

The temperature and residual ionization of the background unperturbed IGM are solved for using RECFAST (Seager, Sasselov & Scott 2000). Fits to the temperature and residual ionization fraction are provided in Appendix A, along with estimates for the expected post-collapse minihalo temperatures.

As galaxies or active nuclei form in the Universe, the radiation from these systems may heat the IGM temperature to higher values. The hydrodynamical models are run without this heat input to provide a reference point for minimal heating. The effect of a warm diffuse IGM on the 21 cm signatures, however, is also explored.

The approach of Bond et al. (1988) is used to describe the collapse of spherical mass shells, with the equations of hydrodynamics solved for numerically. In this paper, the numerical methods of Meiksin (1994) are used. The gas temperature is solved for including atomic collisional and radiative processes, as described in Meiksin (1994), and cooling by molecular hydrogen. The ionization state of the gas is computed as well in order to account for hydrogen recombinations within the halo cores. The computation of molecular hydrogen formation and cooling is described in Appendix C.

At the low-mass end, the baryonic fluctuations are restricted by thermal pressure support, providing a lower limit to the minihaloes which contribute to the 21 cm signal before the fluctuations dissolve into sound waves. It is shown below that the high-mass end is limited by the onset of star formation.

### 3.2 Lower limiting mass

The fluctuations in the baryonic component are filtered at short length-scales by the homogenizing effect of sound waves on scales comparable to the Jeans length. For linear perturbations, the Jeans length is

$$\lambda_J = c_s(rG\rho_M)^{1/2},$$

where $c_s$ is the sound speed in the gas and $\rho_M$ is the total mass density (Peebles 1980). Using the kinetic temperature from equation (A1), this corresponds to a proper Jeans length and total halo mass

$$M_J = (4\pi/3)\rho_M(z)(\lambda_J/2)^3$$

for adiabatic fluctuations at redshift $z$ of

$$\lambda_J \simeq 2.2(1+z)^{-0.525} \text{kpc}; \quad M_J \simeq 220(1+z)^{1.425} M_\odot,$$

(26)

for $6 < z \leq 60$.

The Jeans mass is only an approximation to the lower limiting mass. Lower mass haloes will still contribute a non-negligible 21 cm absorption signal against a bright background radio source distinguishable from the diffuse IGM. As discussed in Section 2.2, the cumulative absorption signal is dominated by the lowest mass haloes still able to retain their gas.

Haloes with masses near the Jeans mass will contribute an emission signal against the CMB provided $T_{\text{b}} > T_{\text{CMB}}$, or $M > 7300 M_\odot$, although with a reduced 21 cm efficiency. An illustrative computation at $z = 20$ is shown in Fig. 1 for a $2.0 \times 10^5 M_\odot$ halo, comparable to the Jeans mass $M_J \simeq 1.7 \times 10^5 M_\odot$. The 21 cm efficiency is appreciable within the core. In fact, the halo mass is below the critical mass required for a shock to form, as given by equation (A7). The gas temperature is determined instead by the adiabatic flow of the gas as it falls into the halo and establishes hydrostatic equilibrium, settling at the binding temperature, equation (A5), within the core. At $z = 20$, the temperature is sufficiently low for $r > 0.8 \text{kpc}$ (comoving) that, from the 21 cm efficiency factor $f_{\text{CMB}}$ given by equation (16), the halo will absorb relative to the CMB rather than emit at these radii. The mass-weighted efficiency within the virial radius, however, still corresponds to net emission, although much reduced from the core value, with $f_{\text{CMB}} \simeq 0.15$. Because of the large number of such small haloes, their net contribution to the 21 cm signatures is non-negligible, particularly at high redshifts.

### 3.3 Upper limiting mass

It has long been suggested that the first collapsing Jeans unstable gaseous structures in a big bang cosmology would have masses of the order of $10^5-10^6 M_\odot$ (Gamow 1948; Peebles & Dicke 1968), with star formation triggered by molecular hydrogen cooling following the formation of $H_2$ through gas phase reactions with $H^-$ and $H^+$ acting as catalysts (Saslaw & Zipoy 1967; Peebles & Dicke 1968; Hirasawa 1969). This picture has survived remarkably well in contemporary cosmological models dominated by cold dark matter, with comparably small masses for the first collapsing objects inferred (Bond & Szalay 1983; Blumenthal et al. 1984; Peebles 1984; Blumenthal et al. 1985; Ostriker & Gnedin 1996; Abel, Bryan & Norman 2000; Fuller & Couchman 2000; Machacek et al. 2001; Reed et al. 2005).

To account for star formation, the creation of molecular hydrogen through gas phase reactions is computed during the collapse (see Appendix C). Only the formation via $H^-$ is included, as the added molecular hydrogen formed via $H_2^+$ is negligible (Palla, Salpeter & Stahler 1983; Lepp & Shull 1984). When the cooling time is shorter than the characteristic inflow time, the gas will be thermally...
unstable (Malagoli, Rosner & Bodo 1987; Balbus & Soker 1989). Overdense pockets of gas are then assumed to cool rapidly and are removed from the flow isochorically (Meiksin 1988). When the cooling time is shorter than the inflow time, mass is removed from the flow and converted into stars at the rate

$$\dot{\rho}_* = q_* \rho / t_{\text{cool}},$$

where $t_{\text{cool}}$ is the net cooling rate within a gas shell, and $q_*$ is a dimensionless efficiency coefficient of order unity.

Once an adequate mass of stars accumulates within a halo, it is presumed that a sufficient number of massive stars will have formed to photoionize the cloud or drive a wind through it via the mechanical energy input from wind losses and supernovae and completely disperse the gas in the cloud. For a Salpeter stellar initial mass function with a minimum stellar mass of 1 M☉ and maximum mass of 100 M☉, an instantaneous burst with a total stellar mass of 10⁶ M☉ formed will produce an ionizing luminosity of 10⁶⁰.8 ph s⁻¹ for a duration of 3.5 × 10⁶ yr, assuming a metallicity of 0.05 solar (Leitherer et al. 1999). Sufficient photons would be produced to photoionize 6 × 10⁶ M☉ of hydrogen, and likely lead to the photoevaporation of the gas in the halo.

Even if radiative recombinations radiated away almost all the photoionization energy, typically at least one star as massive as 50 M☉ will also be produced, corresponding to a massive O-star. Such a star has a lifetime of under 10⁴ yr, after which it will explode as a Type II supernova with a characteristic mechanical energy input of 10⁵¹ erg. Spreading the energy over a characteristic halo baryon mass of 10⁶ M☉ corresponds to a gas temperature of $T_{SN} \simeq 7 \times 10^{6}$ K. Even allowing for 90 per cent of the energy to radiate away, this is more than adequate to unbind the gas. A threshold of 10^7 M☉ is therefore used as a criterion for sufficient star formation to disperse the gaseous content of the halo. It is found that this quantity of stars typically forms soon after the halo collapses. It is also found that the epoch and minimal halo mass for forming sufficient stars to disrupt the halo is not very sensitive to the assumed parameters, such as the star formation efficiency $q_*$ or the minimum required threshold of stars formed.

More generally, an upper limit to the halo mass below which star formation will disrupt a halo may be estimated as follows. After 10^7 yr, the formation of $M_* = 10^5$ M☉ of stars with masses between 1 and 100 M☉ will produce approximately 10^52 erg of mechanical energy in the form of winds and supernovae ejecta (ranging from 10^51.7 to 10^51.9 erg for 0.05 solar to solar metal abundances) (Leitherer et al. 1999). Allowing for a fraction $f_{\text{heat}}$ of this energy to go into heating the gas, and for a fraction $f_b$ of baryons for a total halo mass $M$, setting $(3/2)k_B T_{\text{heat}}/\rho = (f_{\text{heat}}/f_b)(E_3/M)(M_*/1000 M☉)$, where $E_3$ is the mechanical energy input from the formation of 10⁵ M☉ of stars, gives a characteristic gas temperature to which the baryons will be heated

$$T_{\text{heat}} \simeq 2.95 \times 10^5 f_{\text{heat}} E_{3,52} M_{*,3} M_{6}^{-1} \left( \frac{f_b}{0.167} \right)^{-1} K,$$

where $E_{3,52} = E_3/10^{52}$ erg, $M_{*,3} = M_*/10^5$ M☉ and $M_6 = M/10^6 M☉$. Comparison with the binding temperature from equation (A5) gives for the minimum halo mass required to retain the baryons ($T_{\text{heat}} < T_{\text{bound}}$),

$$M_{6,\text{min}} = 137 f_{\text{heat}}^{3/5} \left( \frac{f_b}{0.167} \right)^{-3/5} E_{3,52}^{3/5} M_{*,3}^{3/5} (1 + z_c)^{-3/5}.$$

For $f_{\text{heat}} = 0.5$, at $z_c = 20$ this requires a minimum halo mass of $M > 1.5 \times 10^7 M☉$, corresponding to a post-shock temperature of $T_{\text{sh}} \simeq 9200$ K from equation (A4). This mass is well above the halo masses found below required to form 10^5 M☉ of stars.

Previous estimates of the 21 cm signature have not included the role played by molecular hydrogen cooling, presuming that molecular hydrogen is dissociated by a metagalactic UV radiation field produced by early stars, so that star formation becomes dominated only by more massive ($10^5 - 10^6 M☉$) haloes (Haiman et al. 1997a). Since it is the lower mass haloes that form first, and the gas within them does not survive long once the first stars form within them, it is unclear whether a sufficiently strong radiation field will develop at early epochs. None the less, both models with and without molecular hydrogen formation are considered.

An illustrative computation including molecular hydrogen formation is presented in Fig. 2 for a 1.3 × 10⁶ M☉ halo collapsing at z = 20. The corresponding post-shock temperature is 1770 K from equation (A4), well below the temperature required for collisional ionization. The central temperature in the halo lies below this value because of efficient molecular hydrogen cooling. A comparison run with molecular hydrogen cooling turned off gives a central temperature of $T \simeq 2040$ K. The evolution of the H₂ fraction for the run is shown in Fig. 3, along with the stars formed following H₂ cooling. The column density is computed along lines of sight through a sphere defined by the turn-around radius at each epoch, except at $z = 50$, for which the comoving radius of the initial perturbation is used. It is found that by $z = 20.05$, shortly before the collapse epoch, 10⁵ M☉ of stars has formed for $q_* = 1$.

The entropy generation by the shock just within the turnaround radius results in an inverted entropy profile, as shown in Fig. 2. [The entropy per particle is computed as $s = k_B \log (T^{3/2} n_{\text{H}})$.] The infalling gas may become convectively unstable and the gas turbulent within the core, although the time-scale $t_{\text{inf}} = [(2/3)(g/(s_B))|ds/dr|]^{-1/2}$ (the Brunt–Väisälä time-scale), where g is the gravitational acceleration, is long at these radii. At $z = 20.05$, it is shortest at $r \lesssim 10 kpc$ (comoving), where $t_{\text{inf}} \simeq 69$ Myr. After this time, a spherically symmetric computation will no longer be able to

![Figure 2. Evolution of the fluid variables for a 1.3 × 10⁶ M☉ top that spherical perturbation collapsing at $z_c = 20$. Shown are the hydrogen density (top-left panel), gas temperature (top-right panel), fluid velocity (bottom-left panel) and entropy per particle (bottom-right panel), all as functions of comoving radius. The curves correspond to $z = 50$ (dashed line), $z = 30$ (short-dashed long-dashed line) and $z = 20.05$ (solid line), by which 10⁵ M☉ of stars has formed. The peak temperature at $z = 20.05$ lies somewhat below the predicted post-shock temperature of $T_{\text{sh}} \simeq 1770$ K because of efficient molecular hydrogen cooling.](image-url)
follow the evolution of the system in detail. Because the mechanical energy input by the most massive stars formed will eject the gas on a shorter time-scale, however, the halo will be evacuated before becoming convective. Haloes that reach rapid cooling prior to their collapse redshifts will contribute negligibly to the 21 cm signature by the time the dark matter collapses. This forms a natural upper limit to the mass range of the haloes that do contribute.

The central temperatures found for the collapsing haloes are shown in Fig. 4 for a range of halo masses and redshifts. At low masses, the values with and without molecular hydrogen cooling both agree well with the expected post-shock temperature, as given by equation (A4). Whilst the temperature without molecular hydrogen cooling continues to agree well with the expected post-shock temperature at higher masses, though tending towards the virial temperature, the temperature reaches a ceiling of $T \lesssim 1400$ K when molecular hydrogen cooling is included.

For central temperatures $T \lesssim 8500$ K, atomic cooling through the collisional excitation of Ly$\alpha$ becomes efficient, and stars are presumed to form according to equation (27), as for the case with molecular hydrogen cooling. The breaking of the scaling relation with mass predicted by equation (A4) results in a departure from cosmological self-similar accretion expected in an Einstein–de Sitter universe (Fillmore & Goldreich 1984; Bertschinger 1985). The reasons for the departure are examined in Section 5.6.

In the presence of molecular hydrogen cooling, the maximum halo mass for which fewer than $10^6$ $M_\odot$ of stars form prior to the collapse of the halo is fit to 10 per cent accuracy over $8 < z_\epsilon < 30$ by

$$M_{1000} \simeq 10^6 \left( \frac{26}{1 + z_\epsilon} \right)^{1/2} M_\odot.$$  

This agrees well with fully 3D hydrodynamical simulations of the minimum halo mass of typically $10^7 - 10^8$ $M_\odot$ required for star formation at high redshifts (Abel et al. 2000; Fuller & Couchman 2000; Machacek et al. 2001).

If molecular hydrogen formation is suppressed, higher mass haloes in which Ly$\alpha$ cooling becomes efficient are required for stars to form. In the absence of molecular hydrogen formation, the maximum halo mass for which fewer than $10^7$ $M_\odot$ of stars form prior to the collapse of the halo is fit to 10 per cent accuracy over $8 < z_\epsilon < 50$ by

$$M_{1000}^{\text{noH}} \simeq 9.1 \times 10^6 \exp[-(1 + z_\epsilon)/51] M_\odot.$$  

These masses are about a factor of 5 greater than found when molecular hydrogen cooling is included.

### 3.4 21 cm signature against a bright radio source

The absorption against a bright background source (BBS) is computed from equation (4). An illustration is given in Fig. 5 for a halo with mass $M = 0.9 \times 10^6$ $M_\odot$, including H$_2$ cooling. (The results for the case with H$_2$ cooling suppressed are nearly identical for this mass.) The absorption features are found not to evolve rapidly for a given halo mass, showing only a mild increase in the line centre optical depth with time. The increase results from the continual inflow of material and the departure from self-similar accretion, as discussed below. The trend of increasing optical depth with decreasing collapse epoch is contrary to the redshift scaling expectation for an idealized tophat halo, equation (18), which predicts a decreasing optical depth. The inflow also produces a substantially broader and shallower feature than occurs when the velocity broadening is suppressed.

The profiles shown in Fig. 5 were generated by integrating only along distances within the virial radius of the minihalo. An observed feature would include the absorption by the IGM in the surrounding gas. In Fig. 6, profiles are shown at several impact parameters integrating out to the diffuse IGM. The intergalactic diffuse component is clearly visible in the wings of the features beyond a frequency offset of 4 kHz (in the observed frame). Since individual features
Evolution of the absorption feature against a BBS along a line of sight through the centre of a halo of mass $M = 0.9 \times 10^6 \, M_\odot$, for collapse epochs of $z_c = 15$ (short-dashed line), 10 (long-dashed line) and 8 (solid line). Profiles are shown both including the broadening from the line-of-sight peculiar velocities (heavy lines) and without the peculiar velocity contribution (light lines). The frequency offset from line centre is in the observed frame.

Figure 5. Evolution of the absorption feature against a BBS along a line of sight through the centre of a halo of mass $M = 0.9 \times 10^6 \, M_\odot$, for collapse epochs of $z_c = 15$ (short-dashed line), 10 (long-dashed line) and 8 (solid line). Profiles are shown both including the broadening from the line-of-sight peculiar velocities (heavy lines) and without the peculiar velocity contribution (light lines). The frequency offset from line centre is in the observed frame.

would be measured relative to the diffuse absorption level, the offset at 4 kHz serves as a useful operational definition for the baseline to which the equivalent width of the feature would be determined. This definition for the absorption equivalent width against a BBS will be used throughout the remainder of this paper. According to equation (11), the contribution of a halo of mass $M$ to absorption features with an observed equivalent width exceeding a given $w_{\nu_0}^{\text{obs}}$ scales inversely with the mean free path $\lambda_{\nu_0}^\text{CMB}(w_{\nu_0}^{\text{obs}})$ for intercepting a halo along a line of sight with observed equivalent width exceeding $w_{\nu_0}^{\text{obs}}$. The mean free paths are shown for haloes with $H_2$ cooling collapsing at $z_c = 8$ in Fig. 7 for equivalent width limits $w_{\nu_0}^{\text{obs}} > 0.1, 0.2$ and 0.4 kHz. Most of the systems with $w_{\nu_0}^{\text{obs}} > 0.1$ arise from haloes in the mass range $4 \times 10^7 - 3 \times 10^8 \, h^{-1} M_\odot$.

Figure 7. Comoving mean free path for haloes collapsing at $z_c = 8$ (solid symbols) and $z_c = 10$ (open symbols) for cross-sections giving rise to absorption features against a BBS with observed equivalent widths $w_{\nu_0}^{\text{obs}} > 0.1$ kHz (triangles), $w_{\nu_0}^{\text{obs}} > 0.2$ kHz (squares) and $w_{\nu_0}^{\text{obs}} > 0.4$ kHz (circles).

3.5 21 cm signature against the CMB

The collapsing haloes will produce emission features relative to the CMB. Whilst the signal from an individual halo will not be detectable for the foreseeable future, their profiles reveal the degree to which the signal of a single minihalo may be distinguished from that of the surrounding gas. The temperature differentials in the observed frame are shown in Fig. 8 for a halo with mass $M = 0.9 \times 10^6 \, M_\odot$, including $H_2$ cooling. (The case with $H_2$ cooling suppressed differs little from this mass.) The increase in the brightness temperature for later collapse epochs arises from the continual inflow of material. As in the case for absorption against a BBS, the infall broadens the feature and reduces its amplitude compared with the result when the velocity contribution is suppressed.

Emission against the CMB is not very sensitive to the signature from the infalling gas surrounding the minihalo. This is because collisions are able to decouple the hydrogen spin structure from the CMB only at sufficiently large overdensities near a collapsed halo. The equivalent width weighted cross-section $\Sigma_w^{\text{obs}}$ is only moderately affected by extending the integration volume beyond the core radius, as shown in Fig. 9. Since the mean cosmic optical depth scales in proportion to this factor, as in equation (13), the surrounding gas is not expected to contribute much more to the mean cosmic optical depth. It is the truncation of the signal with impact parameter that provides the justification for treating the minihalo contribution to the total IGM 21 cm signature as distinct from the diffuse component.

The geometrically averaged observed emission equivalent width is shown for a range of halo masses for haloes collapsing at $z_c = 10$ and 20 in Fig. 10. The steep rise in the mean equivalent width with halo mass is partly a consequence of the mass scaling given by equation (22), but is also due to the mass dependence of the 21 cm
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Figure 8. Evolution of the observed brightness temperature relative to the CMB along the line of sight through the centre of a halo of mass \( M = 0.9 \times 10^6 \, M_\odot \); for collapse epochs of \( z_c = 15 \) (short-dashed line), 10 (long-dashed line) and 8 (solid line). Profiles are shown both including the broadening from the line-of-sight peculiar velocities (heavy lines), and without the peculiar velocity contribution (light lines). The frequency offset from line centre is in the observed frame.

Figure 9. Observed integrated equivalent width weighted comoving cross-section for emission against the CMB as a function of comoving maximum impact parameter \( b_{\text{max}} / r_e \), normalized by the core radius. Shown for haloes of mass \( M = 0.9 \times 10^6 \, M_\odot \) (solid lines), \( M = 0.3 \times 10^6 \, M_\odot \) (long-dashed lines) and \( M = 0.8 \times 10^5 \, M_\odot \) (short-dashed lines), for collapse epochs of \( z_c = 8 \) (heavy lines) and 15 (light lines). The turnaround radius corresponds to \( b_{\text{max}} / r_e \approx 3.89 \).

Figure 10. Comoving equivalent width weighted cross-section (in kHz-kpc\(^2\)) for emission against the CMB, as a function of halo mass for haloes collapsing at \( z_c = 10 \) (squares) and \( z_c = 20 \) (circles). The cross-section is shown in the observed frame. Shown for models including \( \text{H}_2 \) cooling (solid symbols) and without (open symbols). Also shown are fits for models without \( \text{H}_2 \) cooling at \( z_c = 10 \) (solid line) and \( z_c = 20 \) (dashed line).

Table 1. Coefficients of \( \Sigma^{\text{wh}}(M) = \Sigma_1^4 c_0 (\log_{10} M)^{d_4} \) for emission against the CMB, for models without \( \text{H}_2 \) cooling. Units are kHz-kpc\(^2\) (comoving).

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4 COSMOLOGICAL 21CM SIGNATURE STATISTICS

4.1 Detection of minihaloes

The models neglect 21 cm absorption or emission from the large-scale surroundings of the minihaloes. As primordial perturbations are intrinsically ellipsoidal (BBKS), and flatten as they grow (Peebles 1980), modelling the region around a minihalo is not straightforward. Only in the late stage of collapse will a spheroidal radiative efficiency \( n_{\text{CMB}} \) of the haloes. The more massive a halo, the greater its 21 cm radiation efficiency for emission against the CMB.

Polynomial fits to the observer-frame equivalent width weighted halo cross-sections of the form \( \Sigma^{\text{wh}} = \Sigma_1^4 c_0 (\log_{10} M)^{d_4} \) are shown as well. The fits are performed for halo masses \( \log_{10} M > 5 \), below which \( \Sigma^{\text{wh}} \) is vanishingly small. Table 1 provides the coefficients for a range of collapse epochs. The fits may be used to interpolate the results of the hydrodynamical models on both the halo mass and the collapse epoch.

The ratios of the equivalent width from the hydrodynamical model to the tophat model for the haloes are shown in Fig. 11. The scaling of the equivalent width with halo mass approaches the tophat prediction for the larger mass haloes. The average values from the hydrodynamical models are much smaller than the tophat prediction from equation (22) at the low-mass end, where the haloes approach the Jeans mass and the gas becomes less overdense, as shown in Fig. 1. The hydrodynamical values agree well with the tophat prediction at the high-mass end despite the very different internal structures of the haloes. The smallest mass haloes actually produce a net absorption signal (cf. Fig. 1).
The degree of spectral isolation of a minihalo may be estimated from the mean free path for intercepting a halo out to the turnaround radius. Approximating the space density of the haloes as $d\nu/d\log M$ gives a mean free path for interception of a typical halo of mass $0.9 \times 10^6 M_\odot$, with a comoving turn-around radius of 12.5 kpc, collapsing at $z_c = 8$ of 3.4 Mpc (comoving). The mean (observed) frequency separation of these systems is about 200 kHz. The detection of an individual absorption feature against a BBS would require measuring the brightness temperature differential within frequency channels not much greater than 8 kHz, and preferably as narrow as 4 kHz or smaller to resolve the feature. For a spectral signal smoothed over broader frequency intervals comparable to the frequency separation of the features, the systems will produce a small modulation of the intensity step from the diffuse gas. For smoothing over much wider frequency intervals, it follows from equation (13) that the contribution from all systems will simply add a small constant amount to the overall intensity step from the diffuse gas.

It is noteworthy that at large redshifts absorption by gas beyond the turnaround radius diminishes $\Sigma^{\rm obs}_{\nu}$ somewhat for emission against the CMB, especially for small mass haloes. As shown in Fig. 9, the asymptotic value of $\Sigma^{\rm obs}_{\nu}$ has not been reached for a $M = 0.8 \times 10^5 M_\odot$ halo collapsing at $z_c = 15$, so that the temperature differential may be somewhat overestimated at these redshifts.

When the 21 cm efficiency of the diffuse component of the IGM exceeds the mass fraction of the IGM in minihaloes, the diffuse IGM signal against the CMB will overwhelm the minihalo signal. Given the mass range of minihaloes that contributes to the minihalo signal, it is possible to estimate the critical Ly$\alpha$ scattering rate required for the diffuse IGM signal to dominate. Using equation (16), and assuming a minimal halo mass given by $M_\delta$, and a maximum mass of $M_{1000}$, or $M_{2000}^{\rm thick}$ if H$_2$ formation is suppressed, produces the critical scattering rates shown in Fig. 12 (upper panel). Only a small fraction of the thermalization rate is required. In fact, for $z > 19$ collisions alone are sufficient to ensure absorption from the diffuse IGM dominates the signal from minihaloes (lower panel). In the presence of moderate amounts of heating, the diffuse IGM will dominate over minihaloes at even smaller redshifts. Shocks in the diffuse IGM may produce further emission against the CMB (Furlanetto & Loeb 2004; Kuhlen et al. 2006; Shapiro et al. 2006).

4.2 21 cm statistics for absorption against a bright radio source

The most readily measured statistic of the minihalo 21 cm signature against a BBS is the equivalent width distribution. The distributions at $z = 8$ and $z = 10$ from the hydrodynamical computations are shown in Fig. 13. The cases with and without H$_2$ cooling have very similar distributions, except that for $z = 8$, the higher mass haloes that survive with H$_2$ formation give rise to a slightly higher frequency of high equivalent width systems, with $w_{\nu_{\rm 21}} > 0.32$ kHz, although these systems are rare.

The distributions are well-fit in the range $0.1 < w_{\nu_{\rm 21}} < 0.3$ kHz by the exponential curve $d^2N/dw_{\nu_{\rm 21}} = N_0 \exp(-w_{\nu_{\rm 21}}/w_0)$. At $z = 8$, $N_0 = 1400$ and $w_0 = 0.069$ kHz, while at $z = 10 N_0 = 3100$ and $w_0 = 0.062$ kHz, both for the case with H$_2$ cooling.

The distribution is dominated by very low mass haloes only for observed equivalent widths below $w_{\nu_{\rm 21}} \lesssim 0.02$ kHz. Excluding haloes with masses no greater than an order of magnitude above the Jeans mass severely suppresses the number of absorption features for such small equivalent width values.

4.3 21 cm statistics for emission against the CMB

The evolution of the observed brightness temperature is shown in Fig. 14. Since the emission equivalent width increases with the mass of the haloes, as shown in Fig. 10, the extension to higher halo...
Figure 13. Observed equivalent width distributions for absorption against a BBS. Top panel: shown are the differential distributions at $z = 8$ (solid lines) and $z = 10$ (dashed lines), with H$_2$ cooling (heavy lines) and without (light lines). The dotted lines show fits through the distributions with H$_2$ cooling. Bottom panel: the corresponding cumulative distributions.

Figure 14. Observed brightness temperature differential relative to the CMB as a function of redshift, including H$_2$ cooling (solid line) and without (dashed line). Masses when H$_2$ formation is suppressed produces a doubling of the differential temperature compared with the case including H$_2$ cooling.

At high redshifts, much of the temperature differential arises from low-mass haloes. Haloes with masses less than an order of magnitude above the Jeans mass contribute about one third of the signal at $z = 20$, both for the cases with and without H$_2$ cooling. The contribution of the low-mass haloes, however, is much reduced by $z = 8$.

The cumulative observed emission equivalent width distributions for haloes collapsing at $z_c = 8$ and 10 are shown in Fig. 15. The heavy curves show the distribution including H$_2$ cooling and the light curves without. The extension to higher mass haloes in the latter case produces a higher frequency of larger equivalent width systems, although the distributions are found to extend to $w_{\text{obs}} > 5$ kHz for both cases. Numerous absorption systems with $-0.01 < w_{\text{obs}} < 0$ kHz arise as well for $z_c = 10$ resulting from absorption in the outer regions of the accreting haloes.

5 DISCUSSION

5.1 21 cm signature statistics

The 21 cm signatures of minihaloes considered here, absorption against a bright background radio source and emission against the CMB, are dominated by haloes in different mass ranges. The absorption signal against a bright source is dominated by haloes in the approximate mass range $4.5 < \log_{10}(M/M_\odot) < 6$. The less massive haloes in this range lie near the Jeans mass, so that the post-infall gas pressure prevents as large an overdensity within the halo core from developing as in the more massive haloes. Haloes with masses above this range have a reduced absorption efficiency as a result of their higher post-shock temperatures. By contrast, the emission signature against the CMB increases with increasing halo mass, limited only by the maximum halo mass before star formation leads to the ejection of the halo gas.

As a consequence of their differing halo mass dependences, the signals will be affected differently by the various parameters defining the models. In this section, the role of some of these parameters in determining the strength of the signals is examined.

An issue only partially addressed in the minihalo approximation is the contribution of the surrounding moderately overdense gas on the overall signals. Minihaloes are not generally isolated structures, but are located within larger scale density inhomogeneities which themselves are non-linear. In the case of absorption against BBSs, the overdense gas surrounding the collapsed minihalo was shown to contribute a small amount to the signal. Because of its near uniformity in frequency, it could be readily subtracted off, leaving the equivalent width largely unaffected.

In the case of emission against the CMB, the role played by the surrounding gas is less clear. Beyond the central emitting minihalo, the gas is sufficiently dense and cool to act as an effective absorber against the CMB, cancelling in part the emission in an unresolved observation. If the absorbing region is sufficiently extensive, it could
substantially reduce the net emission from minihaloes, as has been argued by Kuhlen et al. (2006) on the basis of numerical simulations. It is found here that extending the line-of-sight integration around the minihalo, although producing some reduction in the overall equivalent width, does not reduce it much. It is important to ensure the simulations adequately resolve the minihaloes in extended structures that would appear to be absorbing if under-resolved numerically. Achieving the required resolution in a simulation volume sufficiently large to represent a fair sample of the universe, without itself being overdense, is a formidable computational challenge. A possible solution is to model the statistical fluctuations surrounding the minihaloes semi-analytically.

5.2 Sensitivity to cosmological parameters

A prominent factor in establishing the strength of the signals is the primordial power spectrum. Both 21 cm signatures are sensitive to the amount of power on small scales through their dependence on the halo mass distribution. Indeed, the signatures probe scales smaller than any current measurement of the primordial power spectrum, providing a potentially powerful means of constraining the shape of the primordial power spectrum and even the nature of dark matter.

In Fig. 16, the predicted cumulative observed equivalent width distributions for absorption against a BBS are shown for the best-fitting cosmological models including a running spectral index found by combining WMAP 7 year CMB data with the data from the Atacama Cosmology Telescope (ACT) (Dunkley et al. 2010). Two models are considered. The first is defined by the cosmological parameters \( \Omega_\Lambda = 0.330, \Omega_m = 0.670, \sigma_8/h^2 = 0.02167, h = 0.661, \sigma_{8\nu} = 0.841 \), spectral index at \( k_0 = 0.002 \text{ Mpc}^{-1} \) of \( n(k_0) = 1.032 \) and slope \( d\nu/d\log k = -0.034 \). The second incorporates additional statistical priors based on measurements of the Hubble constant and baryonic acoustic oscillations (BAOs), and is given by the cosmological parameters \( \Omega_\Lambda = 0.287, \Omega_m = 0.713, \Omega_\nu h^2 = 0.02206, h = 0.691, \sigma_{8\nu} = 0.820 \), spectral index at \( k_0 = 0.002 \text{ Mpc}^{-1} \) of \( n(k_0) = 1.017 \) and slope \( d\nu/d\log k = -0.024 \).

The suppression of power on small scales severely reduces the expected number of systems, by as much as two orders of magnitude for the first model. Including the constraints from \( H_0 \) and BAO measurements substantially increases the expected number of systems, but the numbers still lie well below the predictions for the fiducial cosmological model used in this paper. The counts of absorption systems would readily distinguish between the two running spectral index models, illustrating the power the 21 cm detection of minihaloes has for constraining the small-scale primordial density power spectrum in the absence of other suppression mechanisms of the absorbers.

The reduced small-scale power also reduces the predicted temperature differentials from the CMB by factors of a few to several, as shown in Fig. 17. Comparison with Fig. 14 shows the reduction is particularly pronounced at high redshifts. Measurements of the temperature differential especially at high redshift could thus readily constrain the running spectral index in the absence of other sources of suppression of the signal. It is noteworthy that a very weak signal at high redshifts compared with that expected in the fiducial model could be mistaken for a detection of cosmic reionization in the absence of other observational constraints.

The halo mass dependence of the equivalent width for emission against the CMB given by equation (22) suggests the possibility of measuring the halo mass function directly from 21 cm measurements. Whilst the hydrodynamical models produce a diminishing equivalent width with impact parameter, an observation with sufficient angular resolution to resolve the core of the structure could establish the central equivalent width value. The central value is shown as a function of halo mass in Fig. 18. The equivalent width varies with the halo mass approximately as \( w_\nu \sim M^{1.3} \). This is steeper than predicted for the tophat model. None the less, the trend is sufficiently tight to yield a useful measurement of the halo mass.

The opposing mass dependences of the equivalent width as measured in absorption against a BBS, equation (19), and the emission equivalent width in the tophat model, suggests combining them may eliminate the dependence on halo mass, and yield a direct measurement of the combination of cosmological parameters given
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Observed central equivalent width for emission against the CMB collapsing at $w_b = P_{z0} = 0.9 T_{10} (10^{0.9} \text{kpc},$ corresponding to an observed equivalent width $w_{\nu_0} \sim M^{1.3}$.

Figure 18. Observed central equivalent width for emission against the CMB as a function of halo mass, at $z = 10$ (squares), 15 (triangles) and 20 (circles). Results including H$_2$ cooling are shown as solid symbols; open symbols show results without H$_2$ cooling. The dashed line shows power laws $w_{\nu_0} \sim M^{1.3}$.

by

$$\left( \frac{w_{\nu_0}^{\text{obs}}}{w_{\nu_0}^{\text{obs}}}_{\text{BBS}} \right)_{\text{CMB}} \simeq 4.42 \left( \frac{T_{\text{CMB}}}{T_{\text{th}}} \right)^2 \left( \frac{M}{10^9 M_\odot} \right)^2 ( \text{kHz} )^2.$$  

The ratio of equivalent widths eliminates the dependence on the baryon fraction, and would yield a measurement of the halo mass through

$$\left( \frac{w_{\nu_0}^{\text{obs}}}{w_{\nu_0}^{\text{obs}}}_{\text{BBS}} \right)_{\text{CMB}} \simeq 51 \left( \frac{T_{\text{CMB}}}{T_{\text{th}}} \right)^{1/3} \left( \frac{M}{10^9 M_\odot} \right)^{2/3}.$$  

In fact, dissipation breaks these relations. The actual relations both are mass dependent, and have no real mass over inferring the mass from a measurement of the core equivalent width using the scaling relation shown in Fig. 18. Probing the halo cores in emission against the CMB would, of course, be a formidable observational challenge, requiring a space-based facility or possibly one placed on the far side of the Moon to achieve both the required sensitivity free of radio Earthshine (radio-frequency interference) and the long baseline. The larger minihalo cores would just be resolvable within the limitations imposed by image blurring by interplanetary and interstellar plasma, with a characteristic rms spread of $\langle \delta \theta^2 \rangle^{1/2} \simeq 1(\nu/1 \text{ MHz})^{-2} \text{ deg}$ (Carilli 2008).

5.3 Effects of first light

The far-ultraviolet light from the first radiation sources in the Universe will redshift into local Ly$\alpha$ resonance line photons sufficiently distant from the sources. The scattering of the photons off the neutral hydrogen serves as a mechanism to decouple the spin temperature of the hydrogen from the CMB temperature through the Wouthuysen–Field effect (Wouthuysen 1952; Field 1958). Prior to reionization, the intensity will grow sufficiently strong that the Ly$\alpha$ collision rate $P_a$ will approach the thermalization rate $P_{th}$. For a cold IG, with $T_K < T_{\text{CMB}}$, the 21 cm optical depth will increase, increasing the absorption signature of minihaloes against bright background radio sources.

Well before the EoR, a small scattering rate $P_a < P_{th}$ is expected. Whilst the photons will only slightly decouple the spin temperature from the CMB temperature, the vast reservoir of neutral hydrogen outside collapsed haloes will produce a sizeable absorption signature for an IG colder than the CMB (Fig. 12).

Another possible effect of radiation from the first sources is to heat the IGM. Prior to reionization, the primary heating mechanisms are through the photoelectric absorption of X-rays generated in shock-heated collapsed structures, within supernovae remnants from early evolved massive stars, or possibly from any X-ray stellar sources or AGN that have formed (Madau et al. 1997; Tozzi et al. 2000; Carilli et al. 2002; Furlanetto & Loeb 2004; Kuhlen et al. 2006), or by the scattering of higher order Lyman resonance line photons in the vicinity of their sources (Meiksin 2010). The amount of X-ray heating is unknown. Because both 21 cm absorption against a bright radio source and the signal against the CMB are sensitive to the temperature of the IGM, they provide a means of probing the early heating of the IGM by the first radiation sources. Several estimates have been made in the literature for the evolution of the IGM temperature. The model of Furlanetto (2006) is representative, with a heating rate based on the expected amount of star formation at high redshifts, scaling by the low-redshift correlation between X-ray luminosity and star formation in starburst galaxies. The diffuse IGM temperature is found to cross the CMB temperature in the redshift range $12 < z < 15$ for plausible model parameters. By $z = 10$, the IGM temperature is expected to exceed 100 K, and may exceed 1000 K.

An increase in the IGM temperature will have two effects on the 21 cm signatures: an increase in the minimum halo mass giving rise to a signal and the strength of the signal from individual haloes itself. The degree of the hydrodynamical effect on the haloes will depend on the specifics of the heating rate and history. In particular, as discussed in Appendix A, the minimum halo mass required for the gas falling into the halo to shock and virialize increases. In lower mass haloes, the gas is heated by adiabatic compression, and the halo gas density profiles will adjust accordingly. The fraction of haloes affected will increase gradually with the increase in the IGM temperature.

Heating the IGM to a temperature above that of the CMB will produce a qualitative difference in both the absorption signature against a bright background radio source and emission against the CMB since for both cases, dislodging the spin temperature from the CMB temperature through either collisions or Ly$\alpha$ photon scattering will increase the spin temperature. To isolate this latter effect, the spin temperature is re-computed assuming an instantaneous boost of the IGM temperature by $\Delta T_K = 10 T_{\text{CMB}}$, and the impact on the 21 cm signatures assessed. A set of hydrodynamical models with gradual heating is also computed to assess the impact of the hydrodynamical response of the gas on the signal.

5.3.1 21 cm signature against a bright radio source

The spin temperature for the hydrodynamical models is re-computed for five cases, having $P_a/P_{th} = 0.001, 0.01, 0.1, 1$ and 10. Fig. 19 shows typical profiles through a halo of mass $M = 0.9 \times 10^9 M_\odot$ collapsing at $z_c = 10$, including H$_2$ cooling, at a (comoving) projected separation from the halo centre of $b_c = 0.9 \text{kpc}$, corresponding to an observed equivalent width $w_{\nu_0}^{\text{obs}} = 0.20 \text{ kHz}$ for $P_a = 0$. For $P_a = 0.1 P_{th}$, the equivalent width is only slightly reduced. For $P_a = P_{th}$, the equivalent width is nearly halved, to 0.11 kHz. The profile is distorted into one having two minima, one at the central core and the other at the virial radius.
suggestive of two overlapping features. This arises from an enhanced contribution from the outflowing gas beyond the turn-around radius, as shown in Fig. 20. Most of the absorption at \(\nu - \nu_0 = 1\) kHz arises from infalling gas near the centre of the halo (\(x_{\text{com}} < 12.5\) kpc); however the Doppler boosted absorption by outflowing gas also contributes. Whilst the contribution from the outflowing gas is small for \(P_{\text{a}} = 0\), for which the spin temperature is coupled to the CMB temperature, for \(P_{\text{a}} = P_{\text{th}}\) the spin temperature is coupled to the much colder IGM temperature, enhancing the net absorption to beyond that at line centre.

At still larger projected separations, referencing the background continuum to the value at 4 kHz results in positive apparent ‘emission’ features for sufficiently large \(P_{\text{a}}\), as shown in Fig. 21. A line of sight through the halo above at \(b_{\perp} = 5.9\) kpc corresponds to \(w_{\text{obs}}^{\alpha} \approx 0.030\) kHz for \(P_{\text{a}} = 0\). For \(P_{\alpha} = P_{\text{th}}\), the absorption feature would appear as an emission line with \(w_{\text{obs}}^{\alpha} \approx 0.050\) kHz relative to the background absorption level at \(\nu - \nu_0 = 4\) kHz. For \(P_{\text{a}} = 10P_{\text{th}}\), the feature would have \(w_{\text{obs}}^{\alpha} \approx 0.12\) kHz. Such strong mock emission lines against a BBS would be a tell-tale signature of an intense Ly\(\alpha\) background radiation field and a cold IGM.

For a Ly\(\alpha\) scattering rate as large as the thermalization rate, the optical depth increases substantially in the absence of heating, since the IGM temperature is much lower than that of the CMB. As a consequence, weak absorption features along the lines of sight adjacent to low mass haloes become substantially enhanced, resulting in a large number of absorbers. The observed equivalent width cumulative distributions for haloes collapsing at \(z_c = 10\) are shown in Fig. 22 for \(P_{\text{a}} = P_{\text{th}}\) and \(P_{\text{a}} = 10P_{\text{th}}\) (top panel). The (equivalent widths are computed using the intensity at a frequency offset of 2 kHz instead of 4 kHz as the continuum value due to limitations imposed by the volume of the hydrodynamical computations for such high absorption optical depths when \(P_{\text{a}} > P_{\text{th}}\). The distributions are only representative, as features will be produced by much more moderate density fluctuations throughout the IGM, not only in the vicinity of haloes. They indicate, however, the large numbers of features that would arise in a cold IGM.

The mean free path between haloes corresponding to absorption features with observed equivalent widths \(w_{\text{obs}}^{\alpha} < -0.05\) kHz and \(w_{\text{obs}}^{\alpha} > 0.2\) kHz and 0.4 kHz are shown in Fig. 23 (top panel). Systems with \(w_{\text{obs}}^{\alpha} > 0.2\) kHz arise predominantly from low-mass haloes, with a flat contribution over the range \(10^{5} - 10^{6} h^{-1} M_\odot\). Mock emission systems, with \(w_{\text{obs}}^{\alpha} < -0.05\), arise from the outer regions of more massive haloes with masses \(6 - 9 \times 10^{5} h^{-1} M_\odot\).
In an IGM in which \( P_\alpha \) was fluctuating, patches with \( P_\alpha \) exceeding \( P_{th} \) would show up as regions with a highly dense 21 cm forest. Similarly, if \( P_\alpha \) exceeded \( P_{th} \) throughout the IGM while reionization and pre-reionization heating were still incomplete, patches with low \( T_K \) would produce a highly dense 21 cm forest.

The effect of allowing for an instantaneous temperature boost \( \Delta T_K = 10T_{CMB} \) in the IGM on the absorption equivalent width distribution is shown in Fig. 22 (bottom panel) for \( P_{\alpha} = 0, P_{th} \) and \( 10P_{th} \). The effect is to severely reduce the expected number of systems with \( w_{th}^\alpha > 0.1 \) kHz. Weaker features arise predominantly from the peripheries of haloes in the mass range \( 2-5 \times 10^5 h^{-1} M_\odot \), as shown in Fig. 23 (bottom panel). Collisional coupling is weak for this gas, so that the spin temperature is strongly coupled to the CMB temperature and is little affected by a boost in the IGM temperature. The dramatic steepening in the equivalent width distribution would be a means of identifying the presence of a temperature boost.

The mean free path for a feature with \( w_{th}^\alpha > 0.2 \) kHz increases from \( \lambda_{mfp} \simeq 60 h^{-1} \) Mpc (comoving) for \( \Delta T_K = 0 \) and \( P_{\alpha} = 0 \), as shown in Fig. 7, to \( \lambda_{mfp} \simeq 200 h^{-1} \) Mpc (comoving) or larger for \( \Delta T_K = 10T_{CMB} \). The signal is dominated by haloes with a mass \( M \simeq 3 \times 10^7 h^{-1} M_\odot \). Weaker systems, with \( w_{th}^\alpha > 0.1 \) kHz, arise primarily from lower mass haloes, with \( 1-5 \times 10^7 h^{-1} M_\odot \), for \( P_{\alpha} = 0 \). For \( P_{\alpha} = P_{th} \), the signal is dominated by a nearly flat contribution from haloes with masses \( 2 \times 10^5 - 10^7 h^{-1} M_\odot \).

To assess the hydrodynamical impact of a gradual temperature boost, a set of models collapsing at \( z_0 = 10 \), without \( H_2 \) cooling, is computed including a constant photoelectric heating rate per volume by hard photons. The hard radiation field is turned on at \( z = 20 \) with an amplitude adjusted to increase the temperature of the diffuse IGM by \( 10T_{CMB} \) at \( z = 10 \), corresponding to \( T_K \simeq 302 K \) for the diffuse component. Adiabatic compression in a halo with a post-collapse density increase by a factor \( f_c^{-1} \) will heat the collapsed gas to \( f_c^{-2}T_K \), where \( \simeq 9500 K. This greatly exceeds the post-shock temperature of \( T_{th} \simeq 2100 K \), from equation (A4), for a halo as massive as \( M_{th} \simeq 4 \times 10^6 M_\odot \). As a result, the gas temperature increases gradually within the core, and the central density reaches a peak value of a factor of 50 smaller than for the case without external heating, as shown in Fig. 24. The accretion does not establish a steady state, with an outflow from the core developing by \( z = 8 \). The gas density is comparable to the dark matter density within the core at \( z = 10 \), so that a more realistic 3D computation may result in additional compression of the dark matter. The adiabatic heating term, however, would still play an important role in determining the hydrodynamical structure of the halo. The equivalent width along a line of sight passing through the centre of the halo is reduced by a factor of 2.6 compared with the model without external heating, and corresponds to an observed equivalent width of \( w_{obs}^\alpha \simeq 0.13 \) kHz. Higher mass haloes computed are found to produce no larger equivalent widths.

### 5.3.2 21 cm signature against the CMB

The scattering of Ly\( \alpha \) photons weakens the 21 cm emission signature from minihaloes against the CMB as the spin temperature couples increasingly strongly to the lower kinetic temperature of the diffuse IGM. In Fig. 25, the brightness temperature signature is shown for \( P_{\alpha}/P_{th} = 0, 0.01, 0.1 \) and 1. The corresponding observed equivalent widths are \( 9.8, 4.1, -42 \) and \( -270 \) Hz, integrating between \( v - v_0 = \pm 4 \) kHz. The signal is halved for \( P_{\alpha}/P_{th} = 0.01 \), and produces a net absorption signature for \( P_{\alpha}/P_{th} = 0.1 \) and larger.

In fact, the equivalent width of an individual halo is no longer well-defined, since the entire IGM becomes absorbing. From equation (13), the strength of the overall signature depends on the
the minihalo is swamped by the absorption from the surrounding cold IGM. Indeed, on larger scales absorption from the diffuse IGM is expected to dominate, as shown in Fig. 12. For even small values of $P_\alpha/P_{\text{th}}$, the minihalo model is no longer an effective approximation for estimating the signature of the IGM against the CMB. If a direct signal from the minihaloes may be detected at all, it would only be from high angular resolution measurements that were able to resolve individual minihaloes. This would require subarcsecond beam angles, well beyond the specifications of currently existing or planned radio facilities for the foreseeable future.

It is possible that the Ly$\alpha$ scattering rate would be suppressed within dusty regions produced by winds from galaxies, as the Ly$\alpha$ photons would be absorbed along their long path lengths as they re-scatter. In the vicinity of a bright galaxy, however, the scattering of higher order Lyman resonance line photons alone would be adequate to produce a net absorption signature from nearby minihaloes. Typical scattering rates of $P_\alpha/P_{\text{th}} \approx 0.001$–0.01 for Ly-$n$ photons are expected (Meiksin 2010).

Boosting the IGM temperature by $\Delta T_K = 10T_{\text{CMB}}$ gives rise to an emission signature from the diffuse IGM, which produces a wing on the minihalo emission line, as shown in Fig. 27. A substantial emission wing is found even for $P_\alpha = 0$. The collisional coupling to the gas kinetic temperature alone is sufficient to produce the wing (cf. Fig. 12). Even when the frequency range for evaluating the equivalent width is restricted to within 4 kHz of the line centre, the equivalent width weighted cross-section $\Sigma_{w}^{\text{obs}}$ is found not to converge with increasing impact parameter out to at least a few times the turnaround radius, as shown in Fig. 28. Whilst there is a quasi-convergence for $b_\perp \approx r_\odot$, averaging over larger values results in a diverging quantity. The emission signal from the surroundings of the halo swamps that of the minihalo contribution from $b_\perp < r_\odot$. The minihalo model is again no longer a useful approximation for quantifying the contribution to the total temperature differential $T_B - T_{\text{CMB}}$, now dominated by the contribution from the diffuse IGM beyond the core radius of the minihalo.
CMB may be exploited to distinguish the factors of heating, Lyα scattering and the uncertain amount of power on small scales.

In regime (a), absorption by minihaloes against a bright background radio source and emission against the CMB is unaffected by galactic feedback. [By $P_\alpha \ll P_\text{th}$ means a Lyα scattering rate well below that required to increase the 21 cm efficiency of the diffuse component of the IGM to above the mass fraction of the IGM in minihaloes (see Fig. 12.)] The redshift evolution of the signals traces the growth of structures on comoving scales down to a few kiloparsec. In regime (b), the absorption signal against a BBS weakens whilst the minihalo signal against the CMB is largely unaffected. Although the signal from shocked gas in the diffuse IGM may evolve somewhat, it may be possible to isolate the development of large-scale structure using the signal against the CMB from the effects of heating on the absorption systems against bright sources. In regime (c), the signal from the absorption systems weakens as in regime (b), but the signal against the CMB now goes into deep absorption. This would indicate the presence of a moderate metagalactic UV radiation field. Disentangling the effects of heating, Lyα scattering and small-scale power would be difficult. In regime (d), the absorption signal against a BBS continues to diminish as the IGM is warmed, but the signal against the CMB goes into strong emission, which continues to strengthen as either $\Delta T_K$ or $P_\alpha$ increases until the signal saturates with full emission from the IGM against the CMB. Before saturation, joint modelling of the signal against bright sources and against the CMB may partially disentangle the effects of heating, Lyα scattering and small-scale structure growth as an increasing $P_\alpha$ has little effect on the absorption systems but a strong effect on the emission signal against the CMB once $P_\alpha > 0.01 P_\text{th}$. In regime (e), the absorption signal against background sources becomes very strong, producing a large number of absorption systems, whilst the signal from the minihaloes and their environs against the CMB will go strongly into absorption. The large number of absorbers indicates little heating so that its strength is determined primarily by the Lyα scattering rate and the amount of small-scale power. In regime (f), the absorption signal from the minihaloes against a BBS will be diminished, with a large contribution arising from the diffuse IGM. The diffuse IGM signal against the CMB will be in emission and saturate for a sufficiently large Lyα scattering rate. The minihalo signal against the CMB will be overwhelmed by the emission from the diffuse component.

5.4 Effects of reionization

The collapsed haloes achieve large central hydrogen densities and large central H I column densities, with values $N_H > 10^{20}$ cm$^{-2}$ typical. The haloes will be detectable into the EoR, although with reduced cross-sections as their outer regions become heated and photoionized by the ambient UV radiation field. The degree of reduction depends on the intensity of the radiation field.

Two simple limiting cases are considered for estimating the incident flux of ionizing photons. The emissivity necessary for reionizing the Universe may be minimally estimated by requiring one photon per hydrogen atom over a Hubble time. If clumping drives the mean hydrogen recombination time to under a Hubble time, then the emissivity may be estimated instead by requiring one photon per mean hydrogen recombination time. The column density required for shielding the interior of the halo from the incident flux may then be estimated by modelling the ionization zone within the halo as an inverted Strömgren sphere.

The minimal flux based on one photon per baryon is $\langle n_H(z) \rangle c$, where the angle brackets indicate spatial averaging over the IGM.
If the radiation field penetrates to a depth \( l \) within the halo, balancing recombinations with ionizations within the ionized surface layer gives \( \dot{l} \approx (n_{\text{H}}(z))/n_{\text{H}^0}(z) \), where \( n_{\text{H}^0} \) is the internal hydrogen density of the halo and \( \sigma_0 \) the radiative recombination rate (Case B) within the ionized zone. A density of \( n_{\text{H}^0} \) is \( f_c^3 \) and a temperature of \( 10^4 \) K in the ionized layer gives \( N_{\text{H}^0} = n_{\text{H}^0} l = cf_c^3 \sigma_0 \approx 6 \times 10^{20} \text{ cm}^{-2} \) for \( f_c = 1/(18n^2)^{1/3} \). Since the density rapidly rises within the collapsed halo to higher values, the required column density will be somewhat smaller, depending on the mass of the halo and collapse epoch.

If the clumpiness of the IGM is sufficiently large, the ionization will be recombination limited. In this case the incident flux of ionization radiation is \( \langle n_{\text{H}^0} \rangle \sigma_0 c/H(z) \). If the clumping factor of the IGM is dominated by the haloes, then balancing recombinations within the outer ionization layer of a halo with the ionization rate gives a depth for the ionization layer of \( l = f_v c/H(z) \), where \( f_v \) is the volume filling factor of the haloes. For collapsed tophat haloes, this is related to the mass fraction \( f_M \) in collapsed haloes by \( f_v = f_M^2 \). The column density of hydrogen through the ionized layer is then \( N_{\text{H}^0} = f_M n_{\text{H}^0}(z) c/H(z) \approx 10^{22} \text{ cm}^{-2} \) at \( z = 10 \), adopting \( f_M \) from Fig. 12. This means the ionizing radiation would be able to penetrate deeply into the core, much reducing the cross-section, but still not eliminating all the haloes from detection. Many reionization scenarios have been considered in the literature (Gnedin 2000; Ciardi, Stoehr & White 2003; Mellema et al. 2006; Zahn et al. 2007).

5.5 Illustrative detections by radio facilities

The most straightforward means of detecting the 21 cm signature of minihaloes is through absorption against a bright background radio source. Two detection strategies are possible, the direct detection of individual absorption lines and the detection of the ensemble fluctuations produced by the systems. For an absorption feature extending over \( N_{\text{ch}} \) frequency channels of width \( \Delta \omega_{\text{ch}} \), the rms error on the equivalent width is

\[
\langle (\delta w_{\text{obs}}^2) \rangle^{1/2} \approx N_{\text{ch}}^{1/2} \Delta \omega_{\text{ch}} \sigma_{\text{ch}} / l_c,
\]

where \( \sigma_{\text{ch}} \) is the rms instrumental noise level per channel and \( l_c \) is the continuum level of the background radio source.

The expected variance in the measured transmissivity \( Q(\lambda) = \int dx \cdot R(\lambda - \lambda') \exp(-\tau_x) \), where \( R \) describes the response function of the telescope, is given by

\[
\langle (\delta Q)^2 \rangle = \langle (Q - \langle Q \rangle)^2 \rangle = \langle Q \rangle^2 \left[ \int_{-\infty}^{\infty} d\lambda \langle w^2(\lambda) \rangle - 1 \right],
\]

in the limit that the response function is broad compared with the absorption features (Press, Rybicki & Schneider 1993). Here, \( H(\lambda) \) is given by

\[
H(\lambda) = \int_0^\infty \int_0^\infty \int_0^\infty \frac{\partial^3 N}{\partial w_1 \partial \tau_0 \partial \lambda} \times \int_{-\infty}^{\infty} d\lambda' \left[ 1 - e^{-\tau_0^{1/2} \phi_1(\lambda')}] [1 - e^{-\tau_0^{1/2} \phi_1(\lambda'^{-1})} \right],
\]

where \( \partial^3 N/\partial w_1 \partial \tau_0 \partial \lambda \) is the number density of absorption systems per line centre optical depth \( \tau_0 \) per equivalent width (in wavelength) \( w_1 \) per rest wavelength \( \lambda_x = (\lambda - \lambda_0)/(\Delta \lambda_x) \), where \( \Delta \lambda_x = (b(\lambda_0) - \lambda_0) \), and \( \phi_1(\lambda) = \pi^{-1/2} \exp(-\lambda^2) \) is the dimensionless line profile. For \( \tau_0 \ll 1 \), this simplifies to \( H(\lambda) \approx \int d\tau_0 dw_1 \int \partial^3 N / \partial w_1 \partial \tau_0 \partial \lambda \), denoting the number of absorption systems per equivalent width per unit rest wavelength by \( \partial^3 N / \partial w_1 \partial \tau_0 \partial \lambda \). Thus the integration time required to detect the rms fluctuations in the transmissivity arising from the minihaloes is sufficient to detect the stronger absorption features individually. For a longer integration time of 300 h, it would be possible to detect systems down to \( w_{\text{obs}} > 0.05 \) kHz, enabling essentially the full equivalent width distribution to be measured.
only a fraction of the full 48 MHz bandwidth available would be required, allowing the remainder to be used for alternative projects, such as a deep sky survey. As an illustration, for a noise level of $\sigma_A = 6.0 \text{ mJy}$ at 150 MHz in a 12 kHz band for a 1 h integration time, a 5$\sigma$ detection of fluctuations of the magnitude $(\langle \Delta Q^2 \rangle^{1/2} \simeq 0.0028$ against a 6 mJy source at $z = 8$ would require an integration time of 1300 d. Should a source as bright as 30 mJy be found, the integration time shortens to a more manageable 1200 h. For this integration time, it would be possible to detect individual absorption systems four 1 kHz channels wide with $w_{\text{obs}} > 0.18 \text{ kHz}$ at the 5$\sigma$ level.

5.6 Departure from self-similar accretion

The characteristic infall velocity and temperature of the post-shock halo gas predicted from equations (A3) and (A4) (Appendix A) scale as power laws of the halo mass. Self-similar accretion may then be expected, as is the case for cosmological infall of a self-gravitating initially pressureless collisional gas (Bertschinger 1985). A departure from self-similarity, however, is produced by the outer boundary condition of a finite IGM temperature, and so a non-vanishing pressure. Whilst for more massive haloes the IGM pressure may be neglected, the pressure results in a non-negligible contribution to the post-shock temperature in a minihalo.

The jump condition for the temperature for an adiabatic shock is $T_\text{sh} = [2\gamma M_\text{sh}^2 - (\gamma - 1)]([\gamma - 1]M_\text{sh}^2 + 2)/(\gamma + 1)^2 M_\text{sh}^2]$ for a gas with ratio of specific heats $\gamma$, where $M_\text{sh} = |v_\Sigma|/c_\text{s}$ is the Mach number for the inflowing gas with velocity $v_\Sigma$ (relative to the shock front) and adiabatic sound speed $c_\text{s}$. For an initially pressureless gas, the shock is always very strong and the post-shock temperature depends only on the gas velocity, as in equation (A4). For gas starting at the intergalactic temperature, adiabatic compression will pre-warm the gas by a factor of up to $f_{\text{sh}}^{-2}$, as given by equation (A6). This results in a mild shock rather than a strong shock, with the strength of the shock increasing with the halo mass, as shown in Fig. 30. For the larger masses, the post-shock temperature approaches the strong shock limit $T_{\text{sh}}$, of equation (A4) at about half the (proper) collapse radius $r_c = f_{\text{sh}}^{-1} (1 + z)$. As shown in Fig. 30, the gas becomes self-gravitating as the gas continues to flow inwards. For the case of a halo with mass $6 \times 10^9 M_\odot$ (solid curve), the baryonic mass reaches $7 \times 10^9 M_\odot$ in the inner 0.8 kpc (comoving) by $z = 20$, about 50 times the dark matter mass. As the gas comes to rest at the centre of the halo, the gas develops a steep central density profile. The further compression in the time-varying potential results in a further boost in the gas temperature, until values somewhat above $T_{\text{sh}}$ are reached at the centre. In more massive haloes, temperatures approaching, and in some cases even somewhat exceeding, the virial temperature are reached, driving the gas into a rapid cooling phase through Ly$\alpha$ excitation, which will ultimately result in star formation. More than $10^4 M_\odot$ of stars form within the core by $z = 20$. The resulting supernovae will likely expel the gas from the minihalo. A cosmological simulation code unable to resolve the inner few hundred parsecs (comoving) would fail to detect the cooling instability that develops in the centre of the halo, and treat the halo as stable.

One caveat in the solution is that the inverted entropy profile may result in a convective instability outside the core. As discussed in Section 3.3, the growth time is typically longer than the lifetime of massive stars, so that the halo will be disrupted before the instability

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**Figure 29.** The rms fluctuations arising from absorption by minihaloes against a 6 mJy background radio source at $z = 10$, including the instrumental noise contribution, for SKA assuming 10 kHz channels and a 24 h integration time. Shown is the case without feedback, allowing for molecular hydrogen formation (heavy line; solid points) and without (light line; open points). Also shown are several cases with feedback for the model with molecular hydrogen formation at $z = 10$: an instantaneous boost in the IGM temperature by $\Delta T = 10 T_{\text{CMB}}$ with $P_\text{a} = 0$ (solid square) and $P_\text{a} = P_\text{b}$ (solid triangle). The shock shows half the value for the case with $P_\text{a} = P_\text{b}$ and $\Delta T = 0$. Also shown is the case for a gradual increase in the IGM temperature of $\Delta T = 10 T_{\text{CMB}}$ for $z = 10$, including the hydrodynamical response of the gas for a model without H$_2$ formation, with $P_\text{a} = 0$ (open square) and $P_\text{a} = P_\text{b}$ (open triangle). The straight solid line and dashed lines correspond, respectively, to the rms noise level of the telescope in 10 kHz width channels and the rms fluctuations about the noise level averaged over $10^3$ samples in a 10 MHz wide band.
sets in. This will not be the case, however, for haloes of too small mass to form stars. As shown in Fig. 31, the Brunt–Väisälä timescale is shorter than 100 Myr just outside the core radius for the more massive haloes less massive than the critical mass \( \log_{10} M = 6.1 \) for which more than \( 10^5 \) M\(_\odot\) of stars form from H\(_2\) cooling. For the case \( \log_{10} M = 4.73 \), close to the Jeans mass, the gas becomes convectively unstable just within the core. If the timescale is shorter than the typical time between mergers, the halo would become convectively unstable. In this case, the halo gas would fragment, possibly bringing on a contraction of the halo, diminishing the number of systems detected per unit redshift. A high-resolution 3D simulation would be required to assess the effect of the instability.

A second caveat is that the baryons will draw in the dark matter into the central region, an effect not included here. As a consequence, the hydrodynamical flow of the gas must be included to describe the dark matter halo profile on sub-kiloparsec (comoving) scales. The increase in the amount of dark matter will strengthen the gravitational field in the centre of the halo, and enhance the cooling instability.

### 5.7 Comparison with previous results

Fluctuations in the 21 cm signature are an expected consequence of the large-scale structure of the dark matter and baryons in the Universe (Hogan & Rees 1979; Tozzi et al. 2000). The 21 cm forest from small-scale cosmological structures was extracted from numerical reionization simulations by Furlanetto et al. (2002). The IGM was heated by the re-ionizing radiation to a volume-averaged temperature well above that of the CMB, and had a baryonic mass per particle of at best \( \log_{10} M = 5.7 \). The masses of the resolvable dark matter haloes would be over two orders of magnitude larger, exceeding the upper mass limit before stars would form. Most of the features in the simulated spectra in fact arose from moderately overdense filaments, the gas within which will not have been well-resolved into the minihaloes that give rise to the 21 cm features. The simulations were also carried out in boxes too small to provide fair samples of the universe. The simulations none the less clearly established the viability of detecting the 21 cm forest in the spectra of bright background radio sources.

To overcome some of the limitations of simulations, Furlanetto & Loeb (2002) modelled the minihaloes as spheres in hydrostatic equilibrium within a dark matter halo with a static isothermal core at the halo virial temperature and an infalling outer region at the IGM temperature extending to the turn-around radius, beyond which the sphere parameters were adjusted to match on to the diffuse IGM. The IGM temperature from Carilli et al. (2002) was adopted; at \( z = 10 \) the temperature is 1000 K. A model with an IGM temperature a factor 10 lower was also considered. In both cases, the IGM temperature is above the CMB temperature. No models with an IGM temperature lower than that of the CMB were considered. They allow for minihaloes up to a mass corresponding to a virial temperature of \( 10^5 \) K. L\(_{\gamma}\)\(\alpha\) photon scattering rates of \( P_\alpha/P_\gamma \approx 1 \) and 10 at \( z = 10 \) were adopted, as well as \( P_\alpha = 0 \). They find \( dN/dz \approx 10 \) for \( w^{\text{obs}}_\gamma \gtrsim 0.1 \) kHz at \( z = 10 \) for their colder model with \( P_\alpha \approx P_\gamma \). The model parameters correspond closely to those considered here with an instantaneous IGM temperature boost and \( P_\alpha = P_\gamma \). For the model here, \( dN/dz(w^{\text{obs}}_\gamma > 0.1 \) kHz \( ) \approx 1 \), about an order of magnitude smaller. This may in part be due to the somewhat higher IGM temperature of 300 K for the boosted temperature model here, compared with 100 K for the model of Furlanetto & Loeb (2002). Their hotter model, with an IGM temperature of 1000 K, has \( dN/dz(w^{\text{obs}}_\gamma > 0.1 \) kHz \( ) \approx 1 \). In the model here, however, the line density declines faster for systems with \( w^{\text{obs}}_\gamma > 0.3 \) kHz, for which \( dN/dz \approx 0.002 \); Furlanetto & Loeb (2002) obtain 0.02, an order of magnitude larger. The difference may arise from the lower truncation in the upper minihalo mass imposed here, allowing for star formation following H\(_2\) formation. Given the differences between the models, the overall agreement is reasonably good. Of course, as discussed in Section 5.3.1, allowing for the hydrodynamical response of the gas to gradual photoelectric heating corresponding to a temperature boost of \( \Delta T = 10T_{\text{CMB}} \) by \( z = 10 \) eliminates all absorption features with \( w^{\text{obs}}_\gamma > 0.13 \) kHz.
Using a static, non-singular, truncated isothermal sphere model with a temperature given by the virial temperature, and numerical simulations to estimate the halo number density, Shapiro et al. (2006) compute the expected 21 cm emission from minihaloes assuming radiative feedback effects from the first light sources are negligible. They allow for halo masses having virial temperatures up to \(10^5 \text{K} \). At \(z = 8\), they obtain a brightness temperature differential \(\delta T_B = T_B - T_{CMB} \approx 3.5 \text{ mK} \) at \(z = 8\). Adjusting to their cosmological model parameters (similar to those assumed here, except the primordial power spectrum is untilted and normalized to \(\sigma_8 = 0.9\) ), the tophat model for the same mass range predicts \(\delta T_B \approx 3.0 \text{ mK}\), very close to their value. As shown in Fig. 11, however, the tophat model generally exceeds the prediction from the dynamical minihaloes computed here. The dynamical halo model, with \(H_2\) formation suppressed, predicts the smaller value of \(\delta T_B \approx 1.4 \text{ mK} \), allowing for masses up until star formation occurs as given by equation (31). Using the tophat model to extend to the upper mass limit adopted by Shapiro et al. (2006) boosts this value to 1.9 mK. Given the differences between the models, this is reasonably good agreement. The weaker value found here, however, only slightly exceeds the value of 1.5 mK Shapiro et al. (2006) find for the emission from the diffuse IGM alone. Allowing for the lower upper mass limits obtained here suggests the emission from minihaloes is at most comparable to that of the diffuse IGM.

6 SUMMARY AND CONCLUSIONS

A spherical collapse model is used to characterize the 21 cm absorption signatures of minihaloes against bright background radio sources and the CMB prior to the EoR. The model evolves an initially linear spherical perturbation by simultaneously solving for the evolution of the dark matter using a shell code and the gas using a hydrodynamics code. Two sets of models, with and without molecular hydrogen formation, are computed. The resulting models self-consistently include inflow and an accretion shock, and match on to cosmological boundary conditions on large scales. Atomic and molecular radiative processes are included to compute the temperature structure of the haloes. A mass sink is added scaling like \(C_M z^\alpha\) with \(\alpha = 2\), \(C_M = 10\), declining \(\propto C_M z^\alpha\) to a few per unit redshift for observed equivalent widths exceeding 0.25 kHz. Renormalizing to the running spectral index models constrained by both WMAP and ACT CMB data decreases the counts by about 0.5–1 dex, depending on whether or not \(H_\beta\) and baryonic acoustics oscillation constraints are included as well (for which the differences from the WMAP alone results are smaller).

Most of the features arise in haloes with masses between \(10^8\) and \(10^9 M_\odot\). More massive haloes produce fewer absorption features both because they are fewer in number and because of their higher gas temperatures, which act to reduce the optical depth. The full mass range of the haloes that dominates the counts is beyond the reach of current cosmological numerical simulations. The results presented here indicate the mass resolution required to capture the statistics at a given equivalent width limit. Because higher mass haloes do not contribute much to systems with observed equivalent widths between 0.1 and 0.3 kHz, the statistics are fairly insensitive to the role of star formation in limiting the upper mass range of the haloes: results with and without molecular hydrogen formation yield similar results over this equivalent width range.

The observed full width at half-maximum (FWHM) widths of the features are typically 4 kHz, so that the absorption features would be readily resolved in frequency by currently existing or planned radio facilities capable of detecting a cosmological 21 cm signal, given a sufficiently bright background source to build up the required signal-to-noise ratio. Illustrative cases for detections by SKA and LORRF are presented, for both individual absorption lines and the ensemble spectral fluctuations over broad frequency ranges they will induce. It is shown that an observation able to detect the ensemble fluctuations will also detect the stronger individual absorption features, given adequate spectral resolution.

The haloes have typical angular diameters of 0.05–0.25 arcsec at \(z = 10\). Whist the radio core of a quasar is smaller than this, it
is unclear that the dominant radio-emitting region of a background bright radio galaxy would be. The lack of full coverage of the emitting region would reduce the number of absorbers detected. It could alter the equivalent width distribution as well. If the larger haloes giving rise to the larger equivalent width absorbers completely covered the emitting region while the smaller did not, then there would be a large relative reduction in the expected number of weaker equivalent width absorbers. The equivalent width distribution could thus serve as a probe of the size of the emitting regions of radio galaxies.

In a scenario allowing for the production of a metagalactic UV radiation field, a Lyα photon scattering rate matching the thermalization rate, required to decouple the spin temperature from the CMB temperature and begin coupling it to that of the IGM through the Wouthuysen–Field effect, produces absorption features with broad absorption wings. The equivalent width is computed relative to the wings at an observed frequency offset of 4 kHz. In some cases, mock emission lines result relative to the broad absorption wings.

In the presence of Lyα photon scattering at a rate matching or exceeding the thermalization rate $P_{th}$, the number of absorption features is greatly enhanced over the case with no scattering, by more than two orders of magnitude at $z = 10$ for systems with $u^{\text{obs}}_{\text{Lyα}} > 0.15 \text{kHz}$. Increasing the Lyα photon scattering rate to $10P_{th}$, so that the spin temperature is strongly coupled to the IGM temperature everywhere, increases the number of systems with $u^{\text{obs}}_{\text{Lyα}} > 0.25 \text{kHz}$ by three orders of magnitude over the case with no scattering.

Adding a moderate amount of heat to the gas, however, substantially suppresses the number of systems. A sudden temperature boost by 10 times the CMB temperature at $z = 10$ reduces the number of absorption systems with $u^{\text{obs}}_{\text{Lyα}} > 0.2 \text{kHz}$ by about 1 dex in the absence of Lyα photon scattering from the case with no temperature boost. Allowing for a Lyα photon scattering rate 10 times the thermalization rate reduces the number of systems by close to a further order of magnitude. For gradual heating up to 10 times the CMB temperature, adiabatic compressional heating dominates over shock heating within the core, preventing the formation of the high gas density central peak produced in the case without external heating. As a result, absorption features with $u^{\text{obs}}_{\text{Lyα}} > 0.13 \text{kHz}$ are eliminated altogether.

Heating of the IGM is thus degenerate with the suppression of small-scale power in terms of the number of detectable absorption features against a bright background radio source. On the other hand, probing an unheated IGM, even if only the remaining cold patches as heating sources begin to turn on, would result in an unmistakable signal of a cold IGM because of the very large number of absorption systems that result.

For a scenario with no large-scale galactic feedback, the minihaloes will emit relative to the CMB. The individual features have typical observed FWHM widths of 4 kHz, but are unlikely to be resolvable at the signal-to-noise ratio levels achievable in the foreseeable future. Their collective signal, however, may be detectable. Because the strength of the signal of an individual halo increases with the mass of the halo, the overall signal is very sensitive to the assumed maximum halo mass. For models including molecular hydrogen formation, the brightness temperature differential at $z = 15$ is $\delta T_B = T_B - T_{\text{CMB}} \approx 0.2 \text{mK}$, increasing to 0.6 mK at $z = 8$. If molecular hydrogen formation is suppressed, the increase in the upper halo mass raises the signal to 0.4 mK at $z = 15$ and 1 mK at $z = 8$. At these levels, the minihalo signal is comparable to that of the diffuse IGM.

Allowing for a running spectral index constrained jointly by the WMAP and ACT data suppresses the brightness temperature by about a factor of 30 at $z = 15$, and a factor of 5 at $z = 8$, without adding the constraints from $H_0$ and BAO measurements. Adding these constraints reduces the suppression factors to 8 at $z = 15$ and 2–3 at $z = 8$.

The 21 cm signature against the CMB is extremely sensitive to large-scale galactic feedback. Allowing for a metagalactic UV background that produces a Lyα photon scattering rate as small as 1 per cent of the thermalization rate results in an overall absorption signal from the gas within a few times the turn-around radius of the haloes. The overall signature from the minihaloes, including their environment, would be one of absorption.

The absorption signal would weaken as the IGM were heated. Once the IGM temperature exceeds the CMB temperature, however, the opposite effect occurs. Even without Lyα scattering, the emission signal from the gas beyond the core of the halo swamps the signal from within the minihalo core. Allowing for Lyα scattering further increases the strength of emission from the surrounding gas compared with that of the core.

Thus, a minimal amount of galactic feedback, either through the production of Lyα photons or through heating, results in a signal against the CMB from the diffuse IGM that overwhelms that of the minihaloes. The direct measurement of a minihalo signal prior to any galactic feedback would require an absolute calibration of the brightness temperature of a radio telescope to an accuracy of better than $\delta T_B/T_{\text{CMB}} \approx 10^{-4}$ for a detection at $z = 15$. More practical would be an experiment designed to measure the differential brightness temperature between the minihaloes and the CMB by differencing the signals from neutral and ionized patches, either in frequency or in angle on the sky. The circumstances for such a detection, however, would appear to be highly unlikely, perhaps achieved only in the earliest stages of reionization, since the reionization of a large fraction of the IGM would almost certainly be accompanied by galaxy or AGN produced Lyα photons, and possibly heating as well, that would be prevalent throughout the IGM (Madau et al. 1997).

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APPENDIX A: SPHERICAL TOPHAT HALO TEMPERATURE

The temperature (in K) from RECFAST (Seager et al. 2000) is fit to better than 10 per cent accuracy by

\[ T_K = 0.023(1 + z)^{1.95} \] ; 6 < z ≤ 60
\[ = 0.146(1 + z)^{1.50} \] ; 60 < z ≤ 300
\[ = 1.46(1 + z)^{1.10} \] ; 300 < z ≤ 500
\[ = T_{CMB} \] ; z > 500. \hspace{1cm} (A1)

The residual ionization fraction \( n_i / n_{H, tot} \) is fit to better than 5 per cent accuracy by

\[ \frac{n_i}{n_{H, tot}} \times 10^5 = 1.8 + 0.00176(1 + z)^{1.5} \] ; 6 < z ≤ 30
\[ = 2.0 + 0.00082(1 + z)^{1.40} \] ; 30 < z ≤ 100
\[ = 2.0 + 0.00366(1 + z)^{1.1} \] ; 100 < z ≤ 300
\[ = 0.0124(1 + z) \] ; 300 < z. \hspace{1cm} (A2)

The spherical collapse model forms a two-parameter family of solutions for a growing spherical perturbation. A convenient choice for the parameters is the total halo mass and epoch of collapse. For the tophat collapse of a halo of mass \( M \) and comoving radius \( r_0 \), with \( M = (4/3)\pi \rho_{\text{m}}(1+z)^{3} r_0^3 \) where \( \rho_{\text{m}} (z) \) is the total mass density at high redshifts \( z \) when vacuum energy contributes negligibly, the infall velocity \( v_{\text{in}} \) is given by

\[ \frac{1}{2} v_{\text{in}}^2 = \frac{G M}{r_0} = 2 \left( \frac{3\pi}{2} \right)^{2/3} \frac{G M}{r_0} (1 + z_c), \hspace{1cm} (A3) \]

where \( z_c \) is the collapse redshift (Meiksin 2009). The corresponding post-shock gas temperature in the strong shock limit, taking the shock velocity to be \( v_{\text{sh}} \), is given by (for a monatomic gas) \( T_{\text{sh}} = (3/4)T_{\text{virial}} \) where \( (3/2)k_B T_{\text{virial}} = G \bar{m} v_{\text{sh}}^2 / r_0 \), or
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The density fluctuation across it should

\[ T_{ab} = \frac{9}{8} \left( \frac{2\pi^2}{3} \right)^{1/3} \left( 1 + z_c \right) \frac{GM\hat{m}}{k_B r_0} \]

\[ \simeq 1330(1 + z_c) \left( \frac{M/10^9 M_\odot}{r_0/\text{kpc}} \right) K \]

\[ \simeq 72.1(1 + z_c) \left( \frac{M}{10^9 M_\odot} \right)^{2/3} K. \]

where \( \hat{m} \) is the mean mass per particle, assumed to be neutral primordial hydrogen and helium. This is slightly below the nominal mean ‘binding temperature’ of the gas, defined by \((3/2)k_B T_{\text{bind}}/\hat{m} = E_{\text{bind}}/M \simeq (3/5)GM/r_c\), for a baryonic mass in the halo of \( M_h \), and approximating the halo as having uniform density. The temperature may be expressed as

\[ T_{\text{bind}} = \frac{2}{5} \frac{GM\hat{m}}{k_B r_c} = \frac{16}{15} T_{ab} \]

\[ \simeq 76.9(1 + z_c) \left( \frac{M}{10^9 M_\odot} \right)^{2/3} K. \]

These temperatures may be compared with the temperature resulting from the adiabatic compression of the gas in the collapsed halo. For an increase in the gas density by the factor \( \rho_g/\rho_M = f_c^{-3} = 18\pi^2 \), the temperature will increase by the factor \( T_{ab}T_K = (\rho_g/\rho_M)^{2/3} = f_c^{-2} \). Using equation (A1), the resulting adiabatic compression temperature for \( 6 < z_c < 60 \) is

\[ T_{ab} \simeq 0.73(1 + z_c)^{1.95} K. \]

When this temperature exceeds \( T_{ab} \), the gas in the collapsed halo will contract adiabatically rather than shock. This will occur for halo masses smaller than a minimal halo shock mass

\[ M_{ab} \simeq 1020(1 + z_c)^{1.425} M_\odot. \]

If the IGM is heated, \( M_{ab} \) will increase. For example, scaling the unperturbed IGM temperature by the CMB temperature according to \( \Delta T_{\text{CMB}}(z) \) results in the minimum shock mass \( M_{ab} \simeq 1.3 \times 10^9 h^{-1/2} M_\odot \), independent of redshift.

**APPENDIX B: THE MINIHALO MASS FUNCTION**

The density distribution of minihaloes is uncertain. The resolution requirements for an N-body simulation determination are currently too prohibitive to cover the full range of required scales, although progress has been made from very large-scale simulations in estimating the halo number density. A minimum resolution requirement may be estimated as follows. For a simulation to represent a fair amount to resolve Jeans mass haloes.

None the less, substantial progress has been made towards quantifying the abundances of increasingly low-mass haloes. Several such fitting formulas have been presented in the literature, but not down to the halo masses required. The simulations of Reed et al. (2007), however, have reached to \( M \gtrsim 3 \times 10^{10} M_\odot \) at \( z \gtrsim 10 \). They find the halo abundances are described to 4 per cent rms accuracy by the fitting formula

\[ \frac{dn}{dM} = \frac{\Omega_m\rho_c(0)}{\pi^{1/2}M^2} \exp(-t^2)H(n_{\text{eff}}, t) \frac{dt}{d \log M}, \]

where

\[ H(n_{\text{eff}}, t) = 0.542[1 + 0.901t^{-0.6} + 0.6G_1(t) + 0.4G_2(t)] \]

\[ \times \exp \left[ 0.236t^2 - \frac{0.0369}{(n_{\text{eff}} + 3)^{1/2}} \right]. \]

with \( G_1(t) = \exp(-\log t - 0.576)^2/(20.6^2) \), \( G_2(t) = \exp(-\log t - 0.926)^2/(20.2^2) \) and \( n_{\text{eff}} = 6\log d/d\log M - 3 \).

Whilst it is straightforward to extrapolate equation (B1) to the lower masses required, it is unclear how reliable the result would be, especially as the length-scale moves more closely towards the flicker-noise limit for which \( n_{\text{eff}} \approx -3 \). A useful guide may be offered by the density of peaks in a primordial Gaussian dark matter density field, as formulated by BBKS. The density of peaks filtered on a length-scale \( R_t \) is given by

\[ \frac{dn}{dM} = \frac{\Omega_m\rho_c(0)}{\pi^{1/2}M^2} \left( \frac{r}{r_c} \right)^3 \exp(-t^2)G(\gamma, 2^{1/2}\gamma t) \frac{dt}{d \log M}, \]

where \( \gamma = \sigma^2/\langle \sigma_1\sigma_2 \rangle \) and \( r_s = 3^{1/2}\sigma_1/\sigma_2 \) with

\[ \sigma^2(M, z) = \int d \log \, k \Delta^2(k, z)W^2(k, R_t)k^2, \]

\( W(k, R_f) \) is a filter function and \( G \) is a function provided by BBKS. The uncertainty in relating the peaks in the primordial density field to collapsed haloes that form later creates an uncertainty in the relation between the filtering scale \( R_t \) and halo mass \( M \), with, for a Gaussian density profile for example, \( M = (2\pi)^{3/2}\Omega_m\rho_c(0)r_s^3 \), where \( r_s = f_s / R_t \) (Bond & Myers 1996). The BBKS approximation requires fixing \( f_s \), the approach adopted here for its simplicity. More sophisticated approaches allow for the tidal forces that modify the evolution of the primordial perturbations (Bond & Myers 1996), which can be particularly severe for small haloes in the vicinity of larger scale overdensities.

The value for \( f_s \) is found by matching the BBKS approximation to equation (B1) over the mass range \( 3 \times 10^9 < M < 10^9 h^{-1} M_\odot \) at \( z = 10 \) and 20. Choosing a Gaussian filter function \( W \) was found to require a slow variation of \( f_s \) over the mass range. A more effective filter that better describes the structure of haloes is a tophat convolved with an exponential, \( W = W_{\text{th}}W_{\exp} \), where

\[ W_{\text{th}}(k; R_t) = \frac{3}{(kR_t)^2} \left[ \sin(kR_t) - kR_t \cos(kR_t) \right], \]

and

\[ W_{\exp}(k; R_t) = [1 + (0.4kR_t)^2]^{-2} \]

(N. Dalal, Y. Lithwick, M. White, personal communication). Adopting \( \delta_c = 1.683 \) was still found to require a variable \( f_s \), but a constant value is possible choosing instead \( \delta_c = 1.8 \) at \( z = 10 \), with \( f_s = 1.1 \), and \( \delta_c = 1.5 \) at \( z = 20 \), with \( f_s = 0.8 \). The resulting fits are shown in Fig. B1. Better than 15 per cent agreement is found between the BBKS fit and equation (B1) over the mass range \( 3 \times 10^9 < M < 10^9 h^{-1} M_\odot \) at \( z = 10 \), and better than 10 per cent agreement over the mass range \( 3 \times 10^9 < M < 10^9 h^{-1} M_\odot \) at \( z = 20 \). The extrapolation of equation (B1) to \( M_f < M < 3 \times 10^9 h^{-1} M_\odot \) matches the BBKS predictions to better than ~5 per cent at \( z = 10 \) and to better than ~15 per cent at \( z = 20 \). This suggests either relation may be used to estimate the number of minihaloes. In this paper predictions are based on equation (B1).
APPENDIX C: MOLECULAR HYDROGEN FORMATION

C1 Reaction networks

Gas-phase molecular hydrogen production occurs principally through two catalytic processes, via the formation of the intermediates H₋ or H₋₋:

\[ \text{H}^0 + \text{e}^- \rightarrow \text{H}^- + \gamma. \]  
\[ \text{H}^0 + \text{H}^- \rightarrow \text{H}_2 + \text{e}^- \]  
\[ \text{H}^0 + \text{H}^+ \rightarrow \text{H}_2^+ + \gamma. \]  
\[ \text{H}^0 + \text{H}_2^+ \rightarrow \text{H}_2 + \text{H}^+. \]  

Because of the low binding energy of the extra electron in H₋, the reverse of reaction equation (C1) induced by the CMB also becomes important at high redshifts. At high temperatures, the molecular hydrogen may be destroyed through:

\[ \text{H}^0 + \text{H}_2 \rightarrow 3\text{H}^0. \]  

Molecular hydrogen may also be destroyed through collisions with protons (H^+ + H₂ → H₂^+ + H^0), but this will generally be negligible compared with equation (C5) in a largely neutral gas.

For primordial abundances, formation via H₋ generally dominates (Palla et al. 1983; Lepp & Shull 1984). Much more extensive lists of reactions relevant to H₂ formation have been explored, including reactions with deuterium, helium and metals (Glover & Jappsen 2007), but these generally contribute negligibly to the overall abundance of H₂ created in a largely neutral diffuse medium, although they may play roles in the cooling and collapse of a molecular hydrogen cloud. Many of the rates are still poorly determined, and this may affect the rate of cooling and collapse once initiated by a sufficient abundance of molecular hydrogen (Glover & Abel 2008). Since only the formation of sufficient molecular hydrogen to drive cooling is considered here, only the H₋ process is included in the halo collapse models. For the sake of completion, however, the reaction rates involving H₋₋ are listed as well.

C2 Reaction rates

The reaction chain of equations (C1) and (C2) corresponds to the system

\[ \frac{d\rho_{\text{H}^0}}{dt} = k_1 n_{\text{e}^-} n_e - (k_2 n_{\text{H}^0} + k_3) n_{\text{H}^-}, \]  
\[ \frac{d\rho_{\text{H}^-}}{dt} = k_2 n_{\text{H}^0} n_{\text{H}^-} - k_3 n_{\text{H}_2} n_{\text{e}^-}, \]  
where \( n_{\text{H}^0}, n_{\text{H}^-}, n_{\text{H}_2} \) and \( n_e \) are the number densities of H^0, H₋, H₂ and e⁻, respectively. The reaction chain of equations (C3) and (C4) corresponds to the system, including formation by H₋:

\[ \frac{d\rho_{\text{H}^+}}{dt} = k_3 n_{\text{H}^-} n_{\text{H}^0} - k_4 n_{\text{H}_2} n_{\text{e}^-}, \]  
\[ \frac{d\rho_{\text{H}_2^+}}{dt} = k_2 n_{\text{H}^0} n_{\text{H}^-} + k_3 n_{\text{H}_2} n_{\text{e}^-} - k_9 n_{\text{H}_2} n_{\text{e}^-}, \]

where \( n_{\text{H}^-} \) and \( n_{\text{H}_2^+} \) are the number densities of H₋ and H₂^+, respectively.

The reaction rate coefficients used are summarized in Table C1, following the tabelling in Glover & Jappsen (2007). A few comments are required. The rates R1.1a and R1.1b are based on the computation of de Jong (1972), who finds

\[ k_1 \approx 8.92 \times 10^{-7} T^{-3/2} \beta(T), \]

where

\[ \beta(T) = \int_0^k \frac{dk}{(k^2 + 0.0555)} \left[ \exp \left( \frac{15.842}{k^4} \right) - \exp \left( \frac{-0.875}{k^4} \right) \right], \]

where \( T_4 = T/10^4 \) K and k is the wavenumber of the electron in the reverse reaction R51 (photo-detachment). de Jong (1972) tabulates values for \( k_1 \) over \( 10 < T < 15000 \) K. The function \( \beta(T) \) may be approximated as follows. Defining \( x = T_4^{-1} \), \( \beta(T) = y(x)\exp(0.875x) \),

\[ y(x) = \int_0^k \frac{dk}{(k^2 + 0.0555)} \left[ \exp(15.8(k^2 + 0.0555)) - 1 \right]. \]

Differentiating gives

\[ \frac{dy}{dx} = -\frac{15.8 e^{0.875x}}{(15.8x)^{3/2}} \frac{\Gamma(5/2)}{2 \pi^{1/2}} \Phi \left( e^{-0.875x}, \frac{3}{2}, 1 \right), \]

where \( \Phi(\alpha, \beta, 1) = \sum_{n=0}^{\infty} (n+1)^{-\alpha} x^n \) is a Lerch transcendental function. The resulting infinite series representation for \( \beta(T) \) is resummed as a second-order Padé approximant, which is the form provided in Table C1. The expression agrees with the tabulation of de Jong (1972) to better than 1 per cent for \( T < 3000 \) K, and to better than 4 per cent for \( T < 15000 \) K. In the limit \( T \gg 1 \), the rate approaches the asymptotic value \( k_1 \approx 8.92 \times 10^{-13} \Gamma(5/2) \zeta(3/2) [\Gamma(15.8)/15.8]^{-1} \approx 1.64 \times 10^{-15} \text{ cm}^3 \text{ s}^{-1} \), where \( \zeta \) denotes the Riemann \( \zeta \) function. This is the value given by the Padé approximant for \( T \approx 10^4 \) K. An alternative rate, R1.2a and R1.2b, has been provided by Wishart (1979), which agrees reasonably well with de Jong (1972) for \( T < 15000 \) K, and extends the range to higher temperatures. At \( T = 10^4 \) K, it corresponds to \( k_1 \approx 6.34 \times 10^{-15} \text{ cm}^3 \text{ s}^{-1} \), slightly higher than the value given by R1.1a at \( T = 15000 \) K. For this reason R1.1a is fixed at the value at \( T = 15000 \) K (which agrees well with R1.2b at this temperature). The rate for R51 is based on R1.1a assuming the incident radiation is blackbody with a temperature \( T \).
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Table C1. Gas phase reaction rate coefficients \( k_i \) (cm\(^3\)s\(^{-1}\)).

<table>
<thead>
<tr>
<th>No.</th>
<th>Reaction</th>
<th>Rate coefficient</th>
<th>Temperature range</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1.1a</td>
<td>( \text{H}^0 + e^- \rightarrow \text{H}^- + \gamma )</td>
<td>( 1.08 \times 10^{-14} T_{\text{K}}^{\frac{3}{2}} \exp(26.2 + 8.8 T_{\text{K}}) )</td>
<td>( 10 &lt; T &lt; 15000 \text{ K} )</td>
<td>1</td>
</tr>
<tr>
<td>R1.1b</td>
<td></td>
<td>( T_{\text{K}} / 10^3 ), ( z = T_{\text{K}} / 0.875 )</td>
<td>&gt; 15000 K</td>
<td></td>
</tr>
<tr>
<td>R1.2a</td>
<td></td>
<td>( T_{\text{K}} / 10^3 ), ( z = T_{\text{K}} / 0.875 )</td>
<td>T &gt; 6000 K</td>
<td>2</td>
</tr>
<tr>
<td>R1.2b</td>
<td></td>
<td>( T_{\text{K}} / 10^3 ), ( z = T_{\text{K}} / 0.875 )</td>
<td>T &gt; 6000 K</td>
<td>5</td>
</tr>
<tr>
<td>R2.1</td>
<td>( \text{H}^0 + \text{H}^- \rightarrow \text{H}_2 + e^- )</td>
<td>( 1.3 \times 10^{-9} (T/10^3 \text{ K})^{-0.1} )</td>
<td>( 100 &lt; T &lt; 32000 \text{ K} )</td>
<td>3</td>
</tr>
<tr>
<td>R2.2a</td>
<td></td>
<td>( 1.5 \times 10^{-9} )</td>
<td>T &lt; 300 K</td>
<td>4</td>
</tr>
<tr>
<td>R2.2b</td>
<td></td>
<td>( T_{\text{K}} / 10^3 ), ( z = T_{\text{K}} / 0.875 )</td>
<td>T &gt; 300 K</td>
<td></td>
</tr>
<tr>
<td>R3.1</td>
<td>( \text{H}^0 + \text{H}^+ \rightarrow \text{H}_2^+ + \gamma )</td>
<td>( 2.25 \times 10^{-20} \left[ 1 + \frac{7.5 T_{\text{K}}}{(T_{\text{K}}/10^3)^{1/2}} \right] )</td>
<td>( 1 &lt; T &lt; 10^5 \text{ K} )</td>
<td>5</td>
</tr>
<tr>
<td>R3.2</td>
<td></td>
<td>( T_{\text{K}} / 10^3 ), ( z = T_{\text{K}} / 0.875 )</td>
<td>( 10 &lt; T &lt; 3.2 \times 10^5 \text{ K} )</td>
<td>5</td>
</tr>
<tr>
<td>R4.1</td>
<td>( \text{H} + \text{H}_2^+ \rightarrow \text{H}_2 + \text{H}^+ )</td>
<td>( 5.8 \times 10^{-10} )</td>
<td>( T_{\text{K}} / 10^3 ), ( z = T_{\text{K}} / 0.875 )</td>
<td>6</td>
</tr>
<tr>
<td>R4.2</td>
<td></td>
<td>( 1 \times 10^{-10} )</td>
<td>( T_{\text{K}} / 10^3 ), ( z = T_{\text{K}} / 0.875 )</td>
<td>7</td>
</tr>
<tr>
<td>R7.1</td>
<td>( \text{H}^+ + \text{H}_2 \rightarrow \text{H}_2^+ + \text{H}^0 )</td>
<td>( 3 \times 10^{-10} \exp(-21050/T) )</td>
<td>( T_{\text{K}} / 10^3 ), ( z = T_{\text{K}} / 0.875 )</td>
<td>8</td>
</tr>
<tr>
<td>R7.2</td>
<td></td>
<td>( T_{\text{K}} / 10^3 ), ( z = T_{\text{K}} / 0.875 )</td>
<td>( 100 &lt; T &lt; 3 \times 10^4 \text{ K} )</td>
<td>8</td>
</tr>
<tr>
<td>R9.1</td>
<td>( \text{H}^0 + \text{H}_2 \rightarrow 3 \text{H}^0 )</td>
<td>( 1.12 \times 10^{-10} \exp(-70350/T) )</td>
<td>( T_{\text{K}} / 10^3 ), ( z = T_{\text{K}} / 0.875 )</td>
<td>9</td>
</tr>
<tr>
<td>R9.2</td>
<td></td>
<td>( 8.04 \times 10^{-11} T_{\text{K}}^{3/2} \exp(-51790/T)(1 + 0.2130 T_{\text{K}}^{3/2}) )</td>
<td>( 10^3 &lt; T &lt; 10^5 \text{ K} )</td>
<td>10</td>
</tr>
<tr>
<td>R9.3</td>
<td></td>
<td>( T_{\text{K}} / 10^3 ), ( z = T_{\text{K}} / 0.875 )</td>
<td>( T_{\text{K}} / 10^3 ), ( z = T_{\text{K}} / 0.875 )</td>
<td>11</td>
</tr>
<tr>
<td>R51</td>
<td>( \text{H}^- + \gamma \rightarrow \text{H}^0 + e^- )</td>
<td>( 1.04 \times 10^5 T_{\text{K}}^{3/2} \exp(-1/z) )</td>
<td>( T_{\text{K}} / 10^3 ), ( z = T_{\text{K}} / 0.875 )</td>
<td>1</td>
</tr>
</tbody>
</table>


The laboratory measurement of rate R2 at \( T = 300 \text{ K} \) by Martinez et al. (2009) of \( k_2 \approx 2.0 \pm 0.6 \times 10^{-9} \text{ cm}^3 \text{s}^{-1} \) agrees very well with the theoretical value from Dalgaro & Browne (1967) (R2.1), but is also consistent with the somewhat lower value estimated by Launay et al. (1991).

Both R3.1 and R3.2 are fits to the values tabulated in Ramaker & Peek (1976). The fit R3.1 matches the tabulated values to better than 3 per cent for \( 100 < T < 32000 \text{ K} \), decreasing in accuracy at larger values until 17 per cent too small at \( T = 5 \times 10^4 \text{ K} \). Between \( 2 < T < 30 \text{ K} \) the fit is as much as 50 per cent too large. The fit R3.2 matches the tabulated values to within 40 per cent over the range \( 10 < T < 32000 \text{ K} \), and to better than 15 per cent over the range \( 500 < T < 8000 \text{ K} \).

The rate R4.1 agrees well with the value \( k_4 \approx 6.4 \pm 1.2 \times 10^{-10} \text{ cm}^3 \text{s}^{-1} \) measured by Karpas, Anichic & Huntress (1979), but exceeds the alternative rate R4.2 determined by Prasad & Huntress (1980) by a factor of several.

Rate R7 has had a wide range of estimates, as recognized by Savin et al. (2004a), who argue for a similar but more definitive result than provided by Galli & Palla (1998), which is smaller by nearly an order of magnitude compared with the earlier cross-section rough estimate of de Jong (1972).

Rate R9.1 is a fit provided by Shapiro & Kang (1987) to the cross-section values provided by Chernoff, Hollenbach & McKee in a personal communication. It is for hydrogen densities \( n_{\text{H}} \approx 10^{14} \text{ cm}^{-3} \) when \( T < 10^4 \text{ K} \). The rate R9.2 from Dove & Mandy (1986) accounts for quasi-bound states, and is valid for \( n_{\text{H}} < 100 \text{ cm}^{-3} \). The rate R9.3 applies in the low-density limit \( n_{\text{H}} < 1 \text{ cm}^{-3} \) (Lepp & Shull 1983; Mac Low & Shull 1986).

The computations for this paper generally used rates R1.1a, R2.1, R9.2 and R51, although comparison runs were made using some of the alternative rates. The results were not found very sensitive to the choices.

C3 Numerical integration scheme

Despite its simplicity, the system of equations (C6) and (C7) is not straightforward to solve numerically because of the discrepant time-scales between the formation of \( \text{H}^- \) and \( \text{H}_2 \), rendering the system stiff. The solution to the system is

\[
\begin{align*}
\dot{n}_{\text{H}}(t) &= n_{\text{H},0}(t) + [n_{\text{H}}(0) - n_{\text{H},-}(0)] \\
&\times \exp\left[-\int_0^t \! dt' (k_2(t') n_{\text{H},0}(t') + k_{51}(t'))\right] \\
&\times \left[k_2(t') n_{\text{H},0}(t') n_{\text{H},-}(t')\right],
\end{align*}
\]

\[
\begin{align*}
n_{\text{H},0}(t) &= n_{\text{H},0}(0) \exp\left[-\int_0^t \! dt' k_0(t') n_{\text{H},0}(t')\right] \\
&\times \exp\left[-\int_0^t \! dt' k_0(t') n_{\text{H},-}(t')\right] \\
&\times \int_0^t \! dt' \exp\left[-\int_0^{t'} \! dt'' k_0(t'') n_{\text{H},0}(t'')\right] \\
&\times [k_2(t') n_{\text{H},0}(t') n_{\text{H},-}(t')],
\end{align*}
\]

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where \( n_{H^{-}}(t) = k_1(t)n_{He}(t)n_{e}(t)/[k_2(t)n_{e}(t) + k_3(t)] \) is the equilibrium number density of \( n_{H^{-}} \), which is rapidly achieved at high redshifts on the time-scale \( 1/(k_2 n_{e} + k_3) \).

For solving the equations in a homogeneous expanding universe, it is useful to recast them as

\[
\frac{dx_H}{d\tau} = f_{10} - d_{11}x_H; \tag{C16}
\]

\[
\frac{dx_{H_2}}{d\tau} = f_{21}x_H - d_{22}x_{H_2}, \tag{C17}
\]

where \( x_H = n_{H^{-}}/n_{He}, x_{H_2} = n_{H_2}/n_{He}, \) with \( n_{He} \) indicating the total density of hydrogen nuclei in all species, \( f_{10} = k_1 n_{e}/H(\alpha) \), with \( x_{He} = n_{He}/n_{e}, d_{11} = (k_2 n_{e} + k_3)/H(\alpha), \)

\[
f_{21} = k_2 n_{e}/H(\alpha), d_{22} = k_0 n_{e}/H(\alpha), H(\alpha) \text{ is the Hubble constant at epoch } a = 1/(1 + z), \text{ and } \tau = \log a. \text{ The rapidity with which } H^{-} \text{ reaches its equilibrium value suggests the following second-order accurate scheme:}
\]

\[
x_{H^-}^{n+1} = x_{H^-}^n + \left( x_{H^-} - x_{H^-}^0 \right) \times \exp \left[ -\frac{1}{2} \left( d_{11}^n + d_{11}^1 \right) \Delta \tau \right]; \tag{C18}
\]

\[
x_{H_2}^{n+1} = x_{H_2}^n \exp \left[ -\frac{1}{2} \left( d_{22}^n + d_{22}^1 \right) \Delta \tau \right] + \frac{1}{2} \left\{ f_{21}^n x_{H^-}^n \exp \left[ -\frac{1}{2} \left( d_{22}^n + d_{22}^1 \right) \Delta \tau \right] + f_{21}^{n+1} x_{H^-}^{n+1} \right\} \Delta \tau \tag{C19}
\]

for advancing the abundance fractions from time-step \( n \) to \( n+1 = n + \Delta \tau \).

**C4 Effect of molecular hydrogen production on minihaloes**

In this section, the effect of molecular hydrogen production on the collapse of minihaloes is discussed. The large densities in the cores of minihaloes result in rapid cooling either through molecular hydrogen or through collisional excitation of hydrogen. In the presence of molecular hydrogen cooling, the minimum halo mass for forming stars is found to range from 0.9 to \( 1.6 \times 10^6 \, M_\odot \) for \( 30 > z > 8 \), declining to \( 0.4 \times 10^6 \, M_\odot \) at \( z = 50 \). The corresponding range of virial temperatures is \( 3700–1600 \, \text{K} \).

If molecular hydrogen is dissociated by the metagalactic UV radiation field from the first stars, as is argued by Haiman et al. (1997a, 2000), the minimum halo mass for cooling sufficiently to form stars increases to \( 3 \times 10^7–8 \times 10^6 \, M_\odot \) for \( 50 > z > 8 \), corresponding to virial temperatures of \( 14000–4600 \, \text{K} \). This range extends the estimate of \( 10^{13} \, \text{K} \) given by Haiman et al. (2000).

Haiman et al. (2000) argued that only very low UV metagalactic background levels are required to dissociate the molecular hydrogen in haloes with masses below \( 10^7–10^8 \, M_\odot \). The argument was based on hydrostatic minihalo models for which it was presumed that the initial molecular hydrogen content in a halo was negligible. In fact, as shown in Fig. 3, substantial molecular hydrogen formation begins well before collapse, already for overdensities of only a few. A column density of \( N_{H_2} \approx 5 \times 10^{14} \, \text{cm}^{-2} \) is required for self-shielding in a 1000 K halo from an external UV radiation field (Haiman et al. 2000). This is comparable to, but about a factor of 2 larger, than the estimate of de Jong, Boland & Dalgarno (1980) for the required column density for unit optical depth due to Lyman band absorption alone, so that the optical depths shown below may be somewhat underestimated. In the model shown, for which the collapse epoch is \( z_c = 20 \), the molecular hydrogen column density reaches the self-shielding value by \( z = 30 \). Allowing for internal motions, however, may require higher column densities for self-shielding (Glover & Brand 2001).

The fate of early haloes in which molecular hydrogen was formed was also neglected in past computations. These haloes will merge into larger ones, pre-enriching them in molecular hydrogen. The amount of molecular hydrogen within the turn-around radius of non-pre-enriched haloes is shown at the time of their collapse in Fig. C1. This is the amount of molecular hydrogen formed in the diffuse gas.
retained in the halo, as distinct from molecular hydrogen that would form in the gas that becomes thermally unstable and is removed from the halo at the rate $\dot{\rho}_* \propto \rho$ given by equation (27), presumed to form stars. The open symbols correspond to the molecular hydrogen mass within haloes able to form $10^3 M_\odot$ of stars by the time they collapse. Only a small amount of molecular hydrogen need be present to reduce the cooling time sufficiently for the stars to form.

The earlier the collapse epoch, the larger the mass in molecular hydrogen for a given halo mass. Approximating the optical depth to the Lyman–Werner radiation as $\tau_{L-W} \approx (N_{H_2}/5 \times 10^{14}\,\text{cm}^{-2}) (1000K/T)^{1/2}$, Fig. C2 shows that the molecular hydrogen would be self-shielding. A merger event could further concentrate the gas towards the newly formed minihalo centre. Mergers of molecular hydrogen enriched haloes could thus build a substantial reservoir of self-shielded molecular hydrogen clouds within the cores of the minihaloes by the time a substantial UV background develops, lowering the minimum halo mass required for star formation. The topic is worth further investigation with fully 3D computations, including a more complete assessment of the degree to which external Lyman–Werner photons will penetrate the halo core in the presence of velocity gradients within the halo.

As pre-enrichment by mergers was not considered in the models computed here, the minimum halo mass for forming a sufficient number of stars to disrupt the gas in the halo may be even smaller than the models suggest. This would further reduce the numbers of high equivalent width absorption systems along the line of sight to a bright background radio source and weaken the emission signature from minihaloes against the CMB.

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