PROBING THE PRE-REIONIZATION EPOCH WITH MOLECULAR HYDROGEN INTENSITY MAPPING

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Received 2012 December 12; accepted 2013 March 6; published 2013 April 23

ABSTRACT
Molecular hydrogen is now understood to be the main coolant of the primordial gas clouds leading to the formation of the very first stars and galaxies. The line emissions associated with molecular hydrogen should then be a good tracer of the matter distribution at the onset of the reionization of the universe. Here, we propose intensity mapping of H$_2$ line emission in rest-frame mid-infrared wavelengths to map out the spatial distribution of gas at redshifts $z > 10$. We calculate the expected mean intensity and clustering power spectrum for several H$_2$ lines. We find that the 0–0(3) rotational line at a rest wavelength of 9.66 µm is the brightest line over the redshift range of 10–30 with an intensity of about 5–10 Jy sr$^{-1}$ at $z \sim 15$. To reduce astrophysical and instrumental systematics, we propose the cross-correlation between the H$_2$ rotational and vibrational line emission spectrum. Our estimates of the intensity can be used as guidance in planning instruments for future mid-IR spectroscopy missions such as SPICA.

Key words: cosmology: theory – diffuse radiation – intergalactic medium – large-scale structure of universe

Online-only material: color figures

1. INTRODUCTION
Existing cosmological observations show that the reionization history of the universe at $z > 6$ is likely both complex and inhomogeneous (e.g., Haiman 2004; Choudhury & Ferrara 2006; Zaroubi 2012). While the polarization signal in the cosmic microwave background (CMB) anisotropy power spectrum constrains the total optical depth to electron scattering and the existing Wilkinson Microwave Anisotropy Probe measurements suggest reionization happened around $z_{re} = 11$ (Komatsu et al. 2011), it is more likely that the reionization period was extended over a broad range of redshifts from 20 to 6. Moving beyond CMB, observations of the 21 cm spin-flip line of neutral hydrogen are now pursued to study the spatial distribution of the matter content during the epoch of reionization (e.g., Madau et al. 1997; Loeb & Zaldarriaga 2004; Gnedin & Shaver 2004). Unlike CMB, 21 cm data are useful as they provide a tomographic view of the reionization (Furlanetto et al. 2004; Santos et al. 2005). The anisotropy power spectrum of the 21 cm line emission is also a useful cosmological probe (Santos & Cooray 2006; McQuinn et al. 2006; Bowman et al. 2007; Mao et al. 2008).

While the 21 cm signal primarily traces the neutral hydrogen content in the intergalactic medium during reionization, line emission associated with atomic and molecular lines is of interest to study the physical properties within dark matter halos, such as gas cooling, star formation, and the spatial distribution of the first stars and galaxies. Motivated by various experimental possibilities, we have studied the reionization signal associated with the CO (Gong et al. 2011), C II (Gong et al. 2012), and Ly$\alpha$ (Silva et al. 2013) lines. As the signal is sensitive to the metal abundance, these atomic and molecular probes are more sensitive to the late stages of reionization, perhaps well into the epoch when the universe is close to full reionization and has a low 21 cm signal (Basu et al. 2004; Righi et al. 2008; Visbal & Loeb 2010; Carilli 2011; Lidz et al. 2011).

Although the end of the reionization era can be effectively probed with H I, CO, C II, and Lyman-$\alpha$, it would also be useful to have an additional probe of the onset of reionization at $z > 10$. Here we consider molecular hydrogen and study the signal associated with rotational and vibrational lines in the mid-IR wavelengths. Molecular hydrogen has been invoked as a significant coolant of primordial gas leading to the formation of the first stars and galaxies (e.g., Haiman 1999; Bromm & Larson 2004; Glover 2005; Glover 2012). While molecular hydrogen is easily destroyed in the later stages of reionization, its presence in the earliest epochs of the cosmological history can be probed with line emission experiments.

This paper is organized as follows: in the next section, we outline the calculation related to the cooling rate of H$_2$ rotational and vibrational lines. In Section 3, we present results on the H$_2$ luminosity as a function of the halo mass, while in Section 4, we discuss the mean H$_2$ intensity and clustering auto and cross-power spectra. The cross-power spectra between various lines are proposed as a way to eliminate the low-redshift contamination and increase the overall signal-to-noise ratio (S/N) for detection. We discuss potential detectability in Section 5. We summarize our results and conclude in Section 6. We assume the flat LCDM with $\Omega_M = 0.27$, $\Omega_b = 0.046$, $\sigma_8 = 0.81$, $n_s = 0.96$, and $h = 0.71$ for the calculation throughout the paper (Komatsu et al. 2011).

2. H$_2$ COOLING COEFFICIENTS

The radiation emitted by H$_2$ will be generated by the heating/cooling of the gas as the collapsing process evolves. Therefore, in order to calculate the H$_2$ luminosity, we first evaluate the cooling rate of the H$_2$ rotational and vibrational lines for optical-thin and optical-thick media, respectively. For hydrogen density $n_H < 10^3$ cm$^{-3}$, the optical depth is thin for H$_2$ emission lines. Following Hollenbach & McKee (1979), the cooling coefficient for the rotational and vibrational lines can then be expressed as

$$\Lambda_{H_2}^{\nu, \nu}(H_2) = \frac{\Lambda_{LTE}^{\nu, \nu}(H, H_2)}{1 + n_{H_2}^H (H, H_2)/n_{H_2}^H},$$

(1)
where $\Lambda_{\text{LTE}}^{v, \text{rot}}(H, H_2)$ is the cooling coefficients of rotation or vibration at the local thermodynamic equilibrium (LTE) for the collisions with hydrogen atoms $H$ or $H_2$. Here, $n_{\text{LTE}}$ is the critical density of $H$ or $H_2$ to reach the LTE, and $n_{\text{H}, H_2}$ is the local number density of $H$ or $H_2$.

In the LTE, we have $A_J = C_{0J}$, where $A_J$ is the Einstein coefficient, $C_{0J}$ is the collisional de-excitation rate from upper to lower level, and $n$ is the particle number density (Hollenbach & McKee 1979). Then the rotational and vibrational LTE cooling coefficient can be written as

$$
\Lambda_{\text{LTE}}^{v, \text{rot}}(H, H_2) = \frac{1}{n_{\text{H}, H_2}} A_J \frac{g_J}{g_f} e^{-\frac{\Delta E}{kT}} \Delta E,
$$

where $g_J = 2J + 1$ is the statistical weight, $J$ denotes the total angular momentum quantum number of the rotational energy level, $A_J$ is the Einstein coefficient for the $J \rightarrow J'$ transition at the same vibrational energy level or between two vibrational energy levels, and $\Delta E$ is the energy difference between $E_J$ and $E_f$. The wavenumber for each energy level and the calculation for $E_J$ and wavelength are given in the Appendix. The values of $A_J$ are taken from Turner et al. (1977).

Note that we only consider two vibrational level transitions $v = 0$ and 1 in the following calculation. The number of $H_2$ at the highest vibrational levels is much smaller than that at $v = 0$ and 1 in our case, so the strength of these lines is much weaker than those from $v = 0$ and 1. The $n_{\text{crit}}/n$ term in Equation (1) can be approximated by (Hollenbach & McKee 1979)

$$
n_{\text{crit}}^{v, \text{rot}}(H, H_2) = n_{\text{crit}}^{\text{LTE}}(H, H_2) \frac{\Lambda_{\text{LTE}}^{v, \text{rot}}(H, H_2)}{\Lambda_{n, v=0}^{v, \text{rot}}(H, H_2)},
$$

where $n_{\text{crit}}^{v=0}$ is the low-density limit of the cooling coefficient, which can be obtained by replacing the Einstein coefficient in Equation (2) by $C_{0J} n_{\text{H}, H_2}$, i.e.,

$$
\Lambda_{n, v=0}^{v, \text{rot}}(H, H_2) = C_{0J} \frac{g_J}{g_f} e^{-\frac{\Delta E}{kT}} \Delta E.
$$

Here $C_{0J}^{\text{H}, H_2}$ is the collisional de-excitation coefficients with $H$ or $H_2$ for the $J \rightarrow J'$ transition in the same vibrational level or between $v = i$ and $v = j$, which are estimated by the fitting formula given in Hollenbach & McKee (1979) and Hollenbach & McKee (1989; see the Appendix). Using Equations (1)–(4), we can estimate the cooling coefficient for a given $H_2$ line. Note that in Hollenbach & McKee (1979), the fitting formulae of total cooling coefficients for $v = 0$ rotational and $v = 0, 1, 2$ vibrational lines are given. We denote those by $\Lambda_{\text{tot}, \text{rot}}$, $\Lambda_{\text{tot}, \text{vib}}$, and $\Lambda_{\text{tot}, \text{rot,vib}}$ in the cases of the total local, LTE, and low-density limit cooling coefficients, respectively. Then $n_{\text{crit}}/n$ can be expressed by $\Lambda_{\text{tot}} / \Lambda_{\text{tot}, \text{vib}}$, where $n_{\text{crit}}$ denotes the critical density when all energy level transitions are in the LTE.

For the hydrogen density $n_H > 10^3 \text{ cm}^{-3}$, the optical depth is thick for the $H_2$ emission, and we have to consider the absorption effect for the $H_2$ cooling. Following Yoshida et al. (2006), we make use of the cooling efficiency, which is defined by $f_{ce} = \Lambda_{\text{thick}} / \Lambda_{\text{thin}}$ to evaluate the cooling coefficient $\Lambda_{\text{thick}}$ for the optical-thick case. This reduction factor is derived from their simulations and is available for $n_H \lesssim 10^{14} \text{ cm}^{-3}$, which is well within the density ranges of our calculation. The $f_{ce}$ is about 0.02 when $n_H \sim 10^{14} \text{ cm}^{-3}$ and increases to about 0.1 when $n_H \sim 10^{12} \text{ cm}^{-3}$. At densities below $10^{10} \text{ cm}^{-3}$, we have $f_{ce} = 1$ (see Figure 4 of Yoshida et al. 2006).

In Figure 1, as an example, we show the cooling coefficients for $H_2$–$H$ and $H_2$–$H_2$ collisions as a function of temperature $T$. We assume the number density of hydrogen atom $H$ and molecular hydrogen $H_2$ to be $10^7 \text{ cm}^{-3}$ here. The dashed curves show the cooling coefficients of the rotational lines, which are in red (0–0S(0)), magenta (0–0S(1)), green (0–0S(2)), and blue (0–0S(3)). The solid curves are for two vibrational lines 1–0S(1) in red and 1–0Q(1) in blue, respectively. As can be seen, the rotational cooling dominates at the low temperature ($T \lesssim 10^3 \text{ K}$) and the vibrational cooling dominates at high temperature ($T \gtrsim 10^3 \text{ K}$). Also, we find the $\Lambda_{\text{H}_2}$ for $H_2$–$H_2$ collision is generally greater than that for $H_2$–$H$ collision at $T \lesssim 10^3 \text{ K}$, while the $\Lambda_{\text{H}, \text{H}_2}$ for $H_2$–$H$ collision is less than that for $H_2$–$H$ collision in this temperature range. This indicates that at low temperature, the total $\Lambda_{\text{H}, \text{H}_2}$ is mainly from $H_2$–$H_2$ collisions, and the total $\Lambda_{\text{H}, \text{H}_2}$ is from $H_2$–$H$ collisions. At higher temperature with $T \gtrsim 10^3 \text{ K}$, the cooling rates $\Lambda_{\text{H}, \text{H}_2}$ and $\Lambda_{\text{H}, \text{H}_2}$ for both $H_2$–$H$ and $H_2$–$H_2$ collisions are similar.

### 3. H$_2$ Luminosity

We now explore the $H_2$ luminosity as a function of halo mass for rotational and vibrational lines. As discussed in the last section, the $H_2$ cooling coefficient $\Lambda_{\text{H}, \text{H}_2}$ is dependent on the local gas temperature and density of hydrogen and molecular hydrogen. To evaluate $H_2$ luminosity versus halo mass relation for molecular hydrogen cooling within primordial dark matter halos, we first need to know the radial profile of the gas temperature and density within dark matter halos.

Following the results from numerical simulations involving the formation of primordial molecular clouds (e.g., Omukai & Nishi 1998; Abel et al. 2000; Omukai 2001; Yoshida et al. 2006; McGreer & Bryan 2008), we assume the gas density profile as

$$
\rho(r) = \rho_0 \left( \frac{r}{r_0} \right)^{-2.2},
$$

where $\Lambda_{\text{thick}}$ and $\Lambda_{\text{thin}}$ are taken from Turner et al. (1977). Note that we only consider two vibrational level transitions $v = 0$ and 1 in the following calculation. The number of $H_2$ at the highest vibrational levels is much smaller than that at $v = 0$ and 1 in our case, so the strength of these lines is much weaker than those from $v = 0$ and 1. The $n_{\text{crit}}/n$ term in Equation (1) can be approximated by (Hollenbach & McKee 1979)

$$
n_{\text{crit}}^{v, \text{rot}}(H, H_2) = n_{\text{crit}}^{\text{LTE}}(H, H_2) \frac{\Lambda_{\text{LTE}}^{v, \text{rot}}(H, H_2)}{\Lambda_{n, v=0}^{v, \text{rot}}(H, H_2)},
$$

where $n_{\text{crit}}^{v=0}$ is the low-density limit of the cooling coefficient, which can be obtained by replacing the Einstein coefficient in Equation (2) by $C_{0J} n_{\text{H}, H_2}$, i.e.,

$$
\Lambda_{n, v=0}^{v, \text{rot}}(H, H_2) = C_{0J} \frac{g_J}{g_f} e^{-\frac{\Delta E}{kT}} \Delta E.
$$

In Figure 1, as an example, we show the cooling coefficients for $H_2$–$H$ and $H_2$–$H_2$ collisions as a function of temperature $T$. We assume the number density of hydrogen atom $H$ and molecular hydrogen $H_2$ to be $10^7 \text{ cm}^{-3}$ here. The dashed curves show the cooling coefficients of the rotational lines, which are in red (0–0S(0)), magenta (0–0S(1)), green (0–0S(2)), and blue (0–0S(3)). The solid curves are for two vibrational lines 1–0S(1) in red and 1–0Q(1) in blue, respectively. As can be seen, the rotational cooling dominates at the low temperature ($T \lesssim 10^3 \text{ K}$) and the vibrational cooling dominates at high temperature ($T \gtrsim 10^3 \text{ K}$). Also, we find the $\Lambda_{\text{H}_2}$ for $H_2$–$H_2$ collision is generally greater than that for $H_2$–$H$ collision at $T \lesssim 10^3 \text{ K}$, while the $\Lambda_{\text{H}, \text{H}_2}$ for $H_2$–$H$ collision is less than that for $H_2$–$H$ collision in this temperature range. This indicates that at low temperature, the total $\Lambda_{\text{H}, \text{H}_2}$ is mainly from $H_2$–$H_2$ collisions, and the total $\Lambda_{\text{H}, \text{H}_2}$ is from $H_2$–$H$ collisions. At higher temperature with $T \gtrsim 10^3 \text{ K}$, the cooling rates $\Lambda_{\text{H}, \text{H}_2}$ and $\Lambda_{\text{H}, \text{H}_2}$ for both $H_2$–$H$ and $H_2$–$H_2$ collisions are similar.
where we set $r_0 = 1$ pc and $\rho_0$ is the normalization factor which is obtained by

$$M_{\text{gas}} = 4\pi \int_0^{r_{\text{vir}}} r^2 \rho(r) dr. \quad (6)$$

Here, $M_{\text{gas}} = (\Omega_0/\Omega_M) M$ is the gas mass in the virial radius of the halo with dark matter mass $M$, and $r_{\text{vir}}$ is the virial radius which is given by

$$r_{\text{vir}} = \left( \frac{M}{(4/3)\pi \rho_{\text{vir}}} \right)^{1/3}. \quad (7)$$

Here, $\rho_{\text{vir}}(z) = \Delta_c(z) \rho_c(z)$ is the virial density, $\rho_c(z) = 3H^2(z)/(8\pi G)$ is the critical density at $z$, $H(z)$ is the Hubble parameter, and $\Delta_c(z) = 18\pi^2 + 82x - 39x^2$ where $x = \Omega_M(z) - 1$.

We then derive the number density of gas by $n(r) = n_{\text{H}_2}(r) + n_{\text{H}}(r)$. Here, $n_{\text{H}}(r) = f_{\text{H}}(r)/m_\text{H}$ is the number density of hydrogen, where $f_{\text{H}} = 0.739$ is the hydrogen mass fraction and $m_\text{H}$ is the mass of hydrogen atom. Similarly, $n_{\text{H}_2}(r) = 1 - f_{\text{H}}(r)/m_\text{H}$ is the number density of helium, where $m_\text{H}$ is the mass of helium atom. Also, the temperature–density relation $T(n)$ and the $\text{H}_2$ fraction–density relation $f_{\text{H}_2}(n) = n_{\text{H}_2}/n$ can be derived from existing numerical simulations. Here, we use the results on $T(n)$ and $f_{\text{H}_2}(n)$ from Omukai (2001) and Yoshida et al. (2006), which are available for $n \approx 10^{22}–10^{23}$ cm$^{-3}$ as shown in the left panel of Figure 2. The uncertainties of the gas temperature and $\text{H}_2$ fraction are shown in blue regions. These uncertainties are evaluated based on the differences in the far-ultraviolet radiation background from the first stars and quasars (Omukai 2001).

As can be seen, the gas temperature does not monotonously increase with the gas density. For instance, it drops from $T \sim 2000$ to $200$ K between $n \approx 1$ and $10^4$ cm$^{-3}$ where molecular hydrogen density is rising to $f_{\text{H}_2} \sim 10^{-3}$. This indicates that $\text{H}_2$ cooling is starting to become important in this gas density range. At $n \approx 10^4$ cm$^{-3}$, $\text{H}_2$ cooling saturates and turns into the cooling at the LTE. For $n = 10^{10}–10^{11}$ cm$^{-3}$, almost all of the gas particles become molecular hydrogen due to the efficient $\text{H}_2$ three-body reaction (Yoshida et al. 2006), and we find $f_{\text{H}_2} \approx 0.5$ by definition. At $n \approx 10^{20}$ cm$^{-3}$ with $T \approx 10^4$ K, $\text{H}_2$ begins to dissociate and the fraction drops quickly to $f_{\text{H}_2} < 10^{-5}$ when $n \approx 10^{23}$ cm$^{-3}$ and $T \approx 10^4$ K.

Next, with the help of Equation (5), we can evaluate the gas temperature and $\text{H}_2$ fraction as a function of the halo radius, i.e., $T(r)$ and $f_{\text{H}_2}(r)$. Once these are established, we can derive $n_{\text{H}}(r), n_{\text{H}_2}(r)$, and $\Lambda_{\text{H}_2}^{\text{V}}(r)$ which are needed for the $\text{H}_2$ luminosity calculation. In the right panel of Figure 2, we show the density profile of the gas and molecular hydrogen in blue solid and dashed lines for a dark matter halo with $M = 10^8 M_\odot h^{-1}$ at $z = 15$. The blue region shows the uncertainty of the $\text{H}_2$ density profile which is derived by the uncertainty of $f_{\text{H}_2}$ in the left panel of Figure 2. The gas density profile is a straight line with a slope of $-2.2$ as indicated by Equation (5). On the other hand, the density profile of molecular hydrogen has a more complex shape which is dependent on the relation between $f_{\text{H}_2}$ and gas density $n$. For the outer layer of the gas cloud ($r > 10^2$ pc), the gas density is less than $10^5$ cm$^{-3}$ and $f_{\text{H}_2}$ begins to rise up quickly with $n_{\text{H}}$. Here, $f_{\text{H}_2}$ is much smaller than the gas density. For the inner region with $10^{3.5} < r < 10^{-2}$ pc, we find $10^5 < n < 10^{14}$ cm$^{-3}$ and $f_{\text{H}_2}$ begins to rise up quickly with $n_{\text{H}}$, becoming close to the gas density. For the innermost region at $r < 10^{-3.5}$ pc, the gas density is greater than $10^{11}$ cm$^{-3}$, and $f_{\text{H}_2}$ is $0.5$ so that almost all of the hydrogen ends up forming molecular hydrogen.

The luminosity of the $\text{H}_2$ rotational or vibrational lines can then be estimated by

$$L_{\text{H}_2}^{\text{V}}(M, z) = 4\pi \int_{0}^{r_{\text{vir}}} dr r^2 n_{\text{H}_2}^{\text{V}}(r) \times \left[ n_{\text{H}}(r) \Lambda_{\text{H}_2}^{\text{V}}(H) + n_{\text{H}_2}(r) \Lambda_{\text{H}_2}^{\text{V}}(\text{H}_2) \right], \quad (8)$$

where $n_{\text{H}_2}^{\text{V}}(r)$ is the number density of the molecular hydrogen that can emit at a given rotational or vibrational line at $r$. 

\textbf{Figure 2.} Left: the gas temperature $T$ and $\text{H}_2$ fraction $f_{\text{H}_2}$ as functions of the gas density $n$, which are derived from the simulation results in Omukai (2001) and Yoshida et al. (2006). The uncertainties of the gas temperature and $\text{H}_2$ fraction are shown in blue regions. Right: the density profile of the gas (blue solid line) and molecular hydrogen (blue dashed line) for the halo with $M = 10^8 M_\odot h^{-1}$ at $z = 15$. The blue region shows the uncertainty of the $\text{H}_2$ density profile estimated by the uncertainty of $f_{\text{H}_2}$ in the left panel.

(A color version of this figure is available in the online journal.)
We first evaluate the total $n_{H_2}$ at $v = 0$ and 1 states by condensing all the rotational levels at a given vibrational state to be a single vibrational level, $n_i = n_{i-1} \exp[-\Delta E_i/(kT)]$ where $i = 1$. Here, $g_0 = g_1 = 1$ for $v = 0$ and 1, respectively, and $\Delta E_{10}/k \approx 5860$ K (Hollenbach & McKee 1979). Then we estimate $n_{H_2}$ for a given rotational energy level in a vibrational level $i$ by $n_J = n_J \left(g_J/g_{J'}\right) \exp[\Delta E_J/(kT)]$. The fractions of the ortho and para states of total $n_{H_2}$ are assumed to be 0.75 and 0.25, respectively, in our calculation.

In Figure 3, we show the $H_2$ luminosity of several lines as a function of the halo mass at $z = 15$. In these lines, we find that the rotational line 0–0S(3) at a rest-frame wavelength of 9.66 $\mu$m is the most luminous one. Other lines, such as 0–0S(5), 1–0S(1), 1–0Q(1), and 1–0O(3), are also strong for halos with high mass (see also Table 1).

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|c|}
\hline
$H_2$ Line & $\lambda$ (microns) & $\Delta J$ & $A_J$ (s$^{-1}$) & $J_{H_2}$ (Jy sr$^{-1}$) \\
\hline
0–0S(0) & 28.2 & +2 & $2.94 \times 10^{-11}$ & $0.08 \pm 0.06$ \\
0–0S(1) & 17.0 & +2 & $4.76 \times 10^{-10}$ & $1.52 \pm 0.17$ \\
0–0S(2) & 12.3 & +2 & $2.76 \times 10^{-9}$ & $1.32 \pm 0.06$ \\
0–0S(3) & 9.66 & +2 & $9.84 \times 10^{-9}$ & $1.20 \pm 0.03$ \\
0–0S(4) & 8.03 & +2 & $2.64 \times 10^{-8}$ & $0.91 \pm 0.03$ \\
0–0S(5) & 6.91 & +2 & $5.88 \times 10^{-8}$ & $0.77 \pm 0.03$ \\
0–0S(6) & 6.11 & +2 & $1.14 \times 10^{-7}$ & $0.78 \pm 0.03$ \\
0–0S(7) & 5.51 & +2 & $2.00 \times 10^{-7}$ & $1.05 \pm 0.04$ \\
0–0S(8) & 5.05 & +2 & $3.24 \times 10^{-7}$ & $1.31 \pm 0.02$ \\
0–0S(9) & 4.69 & +2 & $4.90 \times 10^{-7}$ & $1.34 \pm 0.01$ \\
0–0S(10) & 4.41 & +2 & $7.03 \times 10^{-7}$ & $1.37 \pm 0.01$ \\
0–0S(11) & 4.18 & +2 & $9.64 \times 10^{-7}$ & $1.39 \pm 0.01$ \\
1–0S(0) & 2.22 & +2 & $2.53 \times 10^{-6}$ & $0.24 \pm 0.07$ \\
1–0S(1) & 2.12 & +2 & $3.47 \times 10^{-6}$ & $3.03 \pm 0.04$ \\
1–0Q(1) & 2.41 & 0 & $4.29 \times 10^{-6}$ & $1.00 \pm 0.01$ \\
1–0O(3) & 2.80 & –2 & $4.23 \times 10^{-7}$ & $0.99 \pm 0.01$ \\
\hline
\end{tabular}
\caption{The Wavelength, $\Delta J = J - J'$, Spontaneous Emission Coefficient $A_J$, Mean Bias, and Mean Intensity for the $H_2$ Rotational and Vibrational Lines at $z = 15$.}
\end{table}

In Figure 4, we show the mean intensity of the most luminous line for 10 $\leq z \leq 30$, and the slopes of the relations for the rotational lines are generally steeper than the vibrational lines. Note that for $5 \leq z \leq 10$ we do not consider the dissociation effect of the molecular hydrogen by Population II and Population III stars. (A color version of this figure is available in the online journal.)

\begin{equation}
\bar{I}_{H_2}(z) = \int_{M_{min}}^{\infty} \frac{dM}{dM} \frac{dn}{dM}(M, z) \frac{L_{H_2}(M, z)}{4 \pi D_L^2} y(z) D_L^2, \quad (9)
\end{equation}

where we choose $M_{min} = 10 M_\odot h^{-1}$, $dn/dM$ is the halo mass function (Sheth & Tormen 1999), $y(z) = d\chi/d\nu = \lambda_{H_2}(1 + z)^2/H(z)$ when $\chi$ is the comoving distance, and $\lambda_{H_2}$ is the wavelength of $H_2$ lines in the rest frame. Our results are not strongly sensitive to the exact value of minimum halo mass. If we increase the minimum halo mass to the level of $10^5 M_\odot h^{-1}$, then the mean intensity we present here decrease by a factor of $\approx 2$ for all $H_2$ lines.

In Figure 4, we show the mean intensity of the eight strongest $H_2$ lines as a function of redshift $z$. The uncertainty in the intensity of the 0–0S(3) line is shown with the shaded blue region, which is derived from uncertainties in the gas temperature and $f_{H_2}$, shown in the left panel of Figure 2. We find that the 0–0S(3) line is the most luminous line for 10 $\leq z \leq 30$, and the slopes of the relations for the rotational lines are generally steeper than the vibrational lines. Note that for $5 \leq z \leq 10$ we do not consider the dissociation effect of the molecular hydrogen by Population II and Population III stars. (A color version of this figure is available in the online journal.)

4. $H_2$ INTENSITY AND POWER SPECTRUM

Given the relation between $H_2$ luminosity and the dark matter halo mass, the mean intensity of the $H_2$ lines can be expressed as (Visbal & Loeb 2010; Gong et al. 2011)

\begin{equation}
\bar{I}_{H_2}(z) = \int_{M_{min}}^{\infty} \frac{dM}{dM} \frac{dn}{dM}(M, z) \frac{L_{H_2}(M, z)}{4 \pi D_L^2} y(z) D_L^2, \quad (9)
\end{equation}

We first evaluate the total $n_{H_2}$ at $v = 0$ and 1 states by condensing all the rotational levels at a given vibrational state to be a single vibrational level, $n_i = n_{i-1} \exp[-\Delta E_{i-1}(kT)]$ where $i = 1$. Here, $g_0 = g_1 = 1$ for $v = 0$ and 1, respectively, and $\Delta E_{10}/k \approx 5860$ K (Hollenbach & McKee 1979). Then we estimate $n_{H_2}$ for a given rotational energy level in a vibrational level $i$ by $n_J = n_J \left(g_J/g_{J'}\right) \exp[\Delta E_J/(kT)]$. The fractions of the ortho and para states of total $n_{H_2}$ are assumed to be 0.75 and 0.25, respectively, in our calculation.
lines are steeper than that of the rotational lines, since they have steeper slopes for cooling coefficients with temperature as shown in Figure 1. However, we find the difference in slopes to become smaller for the rotational lines as J increases, indicating that the high-J rotational lines have similar slopes with cooling coefficient when compared to that of the vibrational lines.

We note here that we do not consider the dissociation effect of the molecular hydrogen by Population II and Population III stars in our calculation. We expect the formation of these stars to be important at $z < 10$ and that there would be a significant amount of H2 that should be dissociated by the UV photons emitting from the first stars. Thus, H2 emission could be suppressed significantly at $z \leq 10$. At $z \sim 15$, there should still be some dissociation but we ignore it to obtain a safe upper limit estimate on the expected H2 intensity for experimental planning purposes.

Next, we can derive the clustering power spectrum of the H2 lines, writing the intensity as $I_{H2}(z) = I_{H2}[1 + b_{H2}(x)]$. Here, $b_{H2}$ is the average H2 clustering bias, which can be estimated from

$$b_{H2}(z) = \frac{\int_{M_{min}}^{\infty} dM \frac{dn}{dM} L_{H2} b(M, z) \int_{M_{min}}^{\infty} dM \frac{dn}{dM} L_{H2}}{\int_{M_{min}}^{\infty} dM \frac{dn}{dM} L_{H2}} ,$$

where $b(M, z)$ is the bias factor for dark matter halos with mass $M$ at $z$ (Sheth & Tormen 1999). The H2 clustering auto power spectrum is then given by

$$P_{H2}^{clus}(k, z) = \frac{2}{H_0^2} P_{H2}^{clus} P_{H2}^{clus}(k, z),$$

where $P_{H2}^{clus}(k, z)$ is the matter power spectrum, which is obtained from a halo model (Cooray & Sheth 2002). At a high redshift as $z = 15$, the structure of matter distribution is extremely linear and the two-halo term dominates the power spectrum.

We can also estimate the shot-noise power spectrum for the H2 lines, which is caused by the discretization of the spacial distribution of the primordial clouds,

$$P_{H2}^{shot}(z) = \int_{M_{min}}^{\infty} dM \frac{dn}{dM} \left[ \frac{L_{H2} y(z) D_A^2}{4 \pi D_L^2} \right]^2 .$$

In Table 1, we tabulate the rest-frame wavelength, $\Delta \lambda = \lambda - \lambda'$, spontaneous emission coefficient $A_j$, mean bias, and mean intensity for 13 rotational and 4 vibrational lines at $z = 15$. The uncertainties of the mean bias and intensity are evaluated by the uncertainty of the gas temperature and $f_{H2}$ from the simulations. We find that the mean intensity of the 0–0(3) rotational line at a rest wavelength of 9.66 $\mu$m is the strongest among these lines, with a value of around 6 Jy sr$^{-1}$ and a range from 3 to 10 Jy sr$^{-1}$. The other rotational lines such as 0–0(5), 0–0(4), 0–0(1), and 0–0(2) are also bright with total intensities of $\sim 4.3, 2.6, 1.2$, and $1.4$ Jy sr$^{-1}$, respectively, at $z = 15$. The vibrational lines 1–0(1), 1–0(2), and 1–0(3) have low mean intensities at the level of 0.83, 1.0, and 0.99 Jy sr$^{-1}$, respectively. The mean bias factor of these lines lies between 2.6 (for 0–0(0)) and 4.2 (for 0–0(11)), and the bias factors of the rotational lines at higher rotational energy level are higher than that at lower level. This is because the lines with high $J$ are stronger at higher mass halos where the temperature is larger.

In the left panel of Figure 5, the clustering auto power spectra of eight H2 lines at $z = 15$ are shown. We find that the shot-noise power spectrum $P_{H2}^{shot}$ is relatively small compared to the clustering power spectrum $P_{H2}^{clus}$, and would not affect $P_{H2}^{clus}$ at the scales of interest. This is easy to understand if we notice that the halo mass function is dominated by halos with low masses which are more abundant.

We also calculate the cross-correlation between two different H2 lines. Such a cross-correlation will reduce the astrophysical contamination from the other sources, such as low-redshift emission lines from star-forming galaxies, including 63 $\mu$m [O I] and 122 $\mu$m [N II], among others. At $z \sim 15$, the dominant rotational line 0–0(3) would be observed at a wavelength of 155 $\mu$m. Such a line would be contaminated by, for example,
\( z \sim 0.3 \) galaxies emitting [N ii]. Thus the auto power spectrum would be higher than what we have predicted given that the line intensities of [N ii] are higher than the H\(_2\) lines. To avoid this astrophysical line confusion, we propose a cross-correlation between two rotational or rotational and vibrational lines of the H\(_2\) line emission spectrum.

The cross-clustering and shot-noise power spectrum for two such H\(_2\) lines \( i \) and \( j \) can be evaluated as

\[
P_{ij}^{\text{class}} = \frac{\bar{P}_{ij} \overline{P}_{ij}}{\sigma_{\text{pix}}^2} P_{\delta \delta}
\]

and

\[
P_{ij}^{\text{shot}} = \int_{M_{\text{min}}}^{\infty} \frac{dM}{dM} \frac{L_{H_2}^i}{4 \pi D_L^2} \frac{L_{H_2}^j}{4 \pi D_L^2} \left( \frac{\bar{y}(z)}{\bar{y}(z)} \right) \left( \frac{\bar{y}(z)}{\bar{y}(z)} \right) D_L^2 D_L,
\]

respectively. From these equations, we find that the cross-power spectrum should have a similar magnitude to the auto power spectrum. The clustering cross-power spectra \( P_{ij}^{\text{class}} \) for several H\(_2\) lines at \( z = 15 \) are shown in the right panel of Figure 5. We choose the strongest 0–0S(3) line to cross-correlate with the other five bright lines, i.e., 0–0S(1), 0–0S(2), 0–0S(4), 0–0S(5), and 1–0Q(1). We find that 0–0S(3) \( \times 0–0S(5) \) is the largest cross-power spectrum since they are brightest two lines. At \( z \sim 15 \), then we would be cross-correlating the wavelength regimes around 110 and 155 \( \mu \)m. A search for mid-IR lines revealed no astrophysical confusions from low redshifts that overlap in these two wavelengths at the same redshift. Thus, while low-redshift lines will easily dominate the auto power spectra of H\(_2\) lines, the cross-power spectrum will be independent of the low-redshift confusions. In addition to reducing the astrophysical confusions, the cross-power spectra also have the advantage that they can minimize instrumental systematics and noise, depending on the exact design of an experiment.

5. DETECTABILITY

In this section, we investigate the possibility of detecting these lines based on current or future instruments. We assume a SPICA-like\(^4\) survey with 3.5 m aperture diameter, 0.1 deg\(^2\) survey area, 10 GHz band width, \( R = 700 \) frequency resolution, 100 spectrometers, and 250 hr total integration time and noise per detector \( \sigma_{\text{pix}} = 10^5 \) Jy \( / \) sr\(^{-1}\) at 100 \( \mu \)m. Such an instrument corresponds to the latest design of the mid-IR spectrometer, BLISS, from SPICA (M. Bradford 2010, private communication).

In Figure 6, we show the errors of the auto power spectrum of the 0–0S(3) line and the cross-power spectrum of 0–0S(3) \( \times 0–0S(5) \) at \( z = 12 \) for two cases, a SPICA/BLISS-like and an experiment with 10\( \times \) better sensitivity than with the current design of SPICA/BLISS with \( \sigma_{\text{pix}} = 10^3 \) Jy \( / \) sr\(^{-1}\). The noise power spectrum from the instrument and shot-noise power spectrum caused by the discrete distribution of the gas clouds are also shown in long-dashed and dotted lines, respectively. We estimate the noise power spectrum and the errors by the same method described in Gong et al. (2012). We find that the S/N is 0.2 and 5.2 for the auto power spectrum of the 0–0S(3) line in the two cases, and S/N = 0.1 and 4.5 for the cross-power spectrum of 0–0S(3) \( \times 0–0S(5) \). This indicates that the current version of SPICA/BLISS does not have the sensitivity to measure the intensity fluctuation of the H\(_2\) lines at a redshift around \( z = 12 \). We find that the noise requirements suggest an instrument that is roughly 10 times better in detector noise than current SPICA/BLISS for a reliable detection.

In addition to measuring the intensity fluctuations, we also explore the detection of the H\(_2\) point sources at high redshifts. In Figure 7, we estimate the number of the H\(_2\) sources for the 0–0S(3) line per deg\(^2\) with flux greater than a given value for three redshift ranges \( 10 \leq z \leq 15 \), \( 15 \leq z \leq 20 \), and \( 20 \leq z \leq 25 \). The uncertainty for \( 10 \leq z \leq 15 \) is shown as an example which is derived from the uncertainties of the simulations. The flux limits of a pencil-beam survey with a SPICA/BLISS-like instrument and a 10\( \times \) better SPICA/BLISS survey for 1\( \sigma \) detection with 250 hr of total integration time are also shown in vertical dash-dotted lines. We find it is hard to detect the H\(_2\) sources even for the redshift range \( 10 \leq z \leq 15 \) using the SPICA/BLISS-like experiment. The number count of

\(^4\) http://sci.esa.int/science-e/www/area/index.cfm?fareaid=105
the $H_2$ sources at $10 \leq z < 15$ is around $10^{-5}$ per deg$^2$ for the SPICA/BLISS-like survey. For the instrument that is $10 \times$ better in sensitivity than SPICA, we find that in this first estimate of $H_2$ counts, we can aim to get about 10 sources per deg$^2$ at $10 \leq z < 15$.

6. DISCUSSION AND CONCLUSION

In this paper, we propose intensity mapping of $H_2$ rotational and vibrational lines to detect the primordial gas distribution at large scales during the pre-reionization epochs at $z > 10$. At such high redshifts, the molecular hydrogen takes the role of main coolant that leads to the formation of the first stars and galaxies and the detection of the $H_2$ power spectrum can reveal details about the halo mass scales which first form stars and galaxies in the universe.

We first estimate the cooling rates for both $H_2$ rotational and vibrational lines with the help of fitting results from Hollenbach & McKee (1979) and Hollenbach & McKee (1989). We find the rotational lines are dominant at low gas temperature, while the vibrational lines are stronger at high gas temperature. Also, the slope of the cooling coefficient–temperature relation for the vibrational lines is steeper than that for the rotational lines. We then derive the gas number density, temperature, and $H_2$ fraction as functions of the halo radius and estimate the relation of the $H_2$ luminosity and halo mass.

Next, we calculate the mean intensity for several $H_2$ lines at different redshifts and find $0-0S(3)$ is the brightest line for $5 \leq z \leq 30$ ($\sim 5.9$ Jy sr$^{-1}$ at $z = 15$). Note that we do not consider the dissociation effects of the $H_2$ by the Population III and Population II stars at $5 \leq z \leq 10$ that could suppress the $H_2$ emission significantly in this redshift range. Finally, we evaluate the clustering and shot noise of the auto and cross-power spectra for the $H_2$ lines at $z = 15$. We find $0-0S(3) \times 0-0S(5)$ is the strongest cross-power spectrum at $z = 15$. We propose such a cross-power spectrum for an experimental measurement as it has the advantage that it can minimize astrophysical line confusion from low-redshift galaxies.

In order to consider potential detection of these mid-IR molecular lines, we evaluate the errors of the $H_2$ auto and cross-power spectrum at $z = 12$ for a SPICA/BLISS-like and a design that is $10 \times$ better than the current instrumental parameters. We find the $S/N$ for the $z = 12$ cross-power spectrum detection is around 0.1 and 5 for these two experiments. We also estimate the detectability of $H_2$ point sources over different redshift ranges. We find that a SPICA/BLISS-like instrument is not able to detect $H_2$ sources for $z > 10$, but an instrument with $10 \times$ better sensitivity than SPICA/BLISS should be able to detect about 10 sources per deg$^2$ for $10 < z < 15$. We encourage further work on this topic to fully account for dissociation as stars and galaxies form and additional formation mechanisms, such as shock heating, that results in $H_2$ line emission from low-redshift galaxies.

This work was supported by NSF CAREER AST-0645427. M.G.S. acknowledges support from FCT-Portugal under grant PTDC/FIS/100170/2008. We thank Matt Bradford for helpful discussions and questions that motivated this paper.

APPENDIX

Here, we list the fitting formulae of the collisional de-excitation coefficients $C_{J}^{H_2}$ for both $H_2$–H and $H_2$–H$_2$ collisions from Hollenbach & McKee (1979) and Hollenbach & McKee (1989). For the rotational cooling in $v = 0$, we have

$$C_{J}^{H_2}(T) = \left( \frac{10^{-11} T_{3}^{0.5}}{1 + 60 T_{3}^{-4}} + 10^{-12} T_{3} \right) \times \left\{ 0.33 + 0.9 \exp \left[ - \left( \frac{J - 3.5}{0.9} \right)^2 \right] \right\} \text{cm}^3 \text{s}^{-1},$$

(A1)

$$C_{J}^{H_2}(T) = (3.3 \times 10^{-12} + 6.6 \times 10^{-12} T_{3}) \times \left\{ 0.276 J^2 \exp \left[ - \left( \frac{J}{3.18} \right)^{1.7} \right] \right\} \text{cm}^3 \text{s}^{-1},$$

(A2)

Figure 7. Number counts of $H_2$ sources for $0-0S(3)$ line, per deg$^2$ with flux greater than a given value for different redshift ranges. The uncertainty for $z = 10-15$ is shown in blue region, which is estimated by the uncertainties of the gas density and $n_H$. We also show the flux limit of a SPICA/BLISS pencil-beam survey and another with $10\times$ better instrumental sensitivity, for a 1σ detection with 250 hr of integration time.

(A color version of this figure is available in the online journal.)

Table 2

The Wavenumbers in cm$^{-1}$ of $H_2$ Energy Levels for $J = 0, \ldots, 13$ at $v = 0$ and 1

| $J$ | $\nu = 0$ | $\nu = 1$ |
|-----|-----------|-----------|
| 0   | 0.00      | 4161.14   |
| 1   | 118.50    | 4273.75   |
| 2   | 354.35    | 4497.82   |
| 3   | 705.54    | 4831.41   |
| 4   | 1168.78   | 5271.36   |
| 5   | 1740.21   | 5813.95   |
| 6   | 2414.76   | 6454.28   |
| 7   | 3187.57   | 7187.44   |
| 8   | 4051.73   | 8007.77   |
| 9   | 5001.97   | 8908.28   |
| 10  | 6030.81   | 9883.79   |
| 11  | 7132.03   | 10927.12  |
| 12  | 8298.61   | 12031.44  |
| 13  | 9523.82   | 13191.06  |
where \( T_3 = T/1000 \) K and \( T \) is the gas temperature. For the vibrational cooling between \( v = 1 \) and 0, we have
\[
C_{10}^{\text{H}}(T) = 1.0 \times 10^{-12} T^{0.5} \exp[-(1000/T)] \text{cm}^3 \text{s}^{-1},
\]  
\( \text{(A3)} \)
\[
C_{10}^{\text{H}_2}(T) = 1.4 \times 10^{-12} T^{-0.5} \exp[-18100/(T + 1200)] \text{cm}^3 \text{s}^{-1}.
\]  
\( \text{(A4)} \)

The wavenumbers \( k = 1/\lambda \) of the \( \text{H}_2 \) energy levels for \( J = 0, \ldots, 13 \) at \( v = 0 \) and 1 from Dabrowski (1984) are listed in Table 2. We can get the energy for each level by \( E_J = h \nu c \), where \( h \nu \) is the Planck constant and \( c \) is the speed of light. The wavelengths of the \( \text{H}_2 \) line hence could be derived by \( \lambda_{\text{H}_2} = h \nu c/(E_J - E_{J'}) \).