OXYGEN PUMPING: PROBING INTERGALACTIC METALS AT THE EPOCH OF REIONIZATION

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ABSTRACT

We consider the pumping of the 63.2 μm fine-structure line of neutral O i in the high-redshift intergalactic medium (IGM), in analogy with the Wouthuysen-Field effect for the 21 cm line of cosmic H i. We show that the soft UV background at ~1300 Å can affect the population levels, and if a significant fraction of the IGM volume is filled with “fossil H II regions” containing neutral O i, then this can produce a nonnegligible spectral distortion in the cosmic microwave background (CMB). O i from redshift z is seen in emission at (1 + z)63.2 μm, and in the range 7 < z < 10 produces a mean spectral distortion of the CMB with y = (10^{-9} to 3 \times 10^{-8})Z(10^{-2}Z_{\odot})/(10^{-8}Z_{\odot}), where Z is the mean metallicity of the IGM and I_H is the UV background at 1300 Å in units of 10^{-20} ergs s^{-1} Hz^{-1} cm^{-2} sr^{-1}. A measurement of this signature can trace the metallicity at the end of the dark ages, prior to the completion of cosmic reionization, and is complementary to cosmological 21 cm studies. While future CMB experiments such as Planck could constrain the metallicity to the 10^{-2}Z_{\odot} level, specifically designed experiments could potentially achieve a detection.

Subject headings: cosmic microwave background — cosmology: theory — intergalactic medium — ISM: abundances

The first sources of light that ended the cosmic dark ages are expected to have reionized the intergalactic medium (IGM) and polluted it with metals (e.g., Loeb & Barkana 2001). To use the metal enrichment as a potential probe of the reionization epoch, recent studies have concentrated on the neutral oxygen (O i) produced by the first massive stars (Oh 2002; Basu et al. 2004).

The ionization potential of O i is only 0.2 eV higher than that of hydrogen (H i), and the two species are in charge exchange equilibrium. Therefore, oxygen is likely to be highly ionized in regions of the IGM where hydrogen is ionized. However, the recombination time for oxygen (as for hydrogen) is shorter than the Hubble time at z ≥ 6, indicating that oxygen can be neutral even in regions where H has been ionized but where short-lived ionizing sources have turned off, allowing the region to recombine (Oh 2002). Numerical simulations that do not resolve the first generation of “minihalos” find a small volume filling factor of such “fossil” H II regions (Iliev et al. 2007; McQuinn et al. 2006; Ricotti et al. 2002).

However, Oh & Haiman (2003) argued, in a semianalytical model, that minihalos are more susceptible to negative feedback and that they can produce fossil H II regions that occupy >50% of the volume of the IGM prior to reionization. More generally, the distribution of metals around early galaxies is poorly understood, but they may preferentially occupy denser regions around galaxies, where recombination time is short (Theuns et al. 2002; Miralda-Escudé et al. 2000; Cen & Ostriker 1999). Moderate wind velocities (10–100 km s^{-1}) suffice to pollute a significant fraction of the IGM volume, in principle (Haiman 2003), although the metal escape can be hindered by large-scale structures around the small galaxies. In fact, Becker et al. (2006) claim to have found evidence for significant O i absorption in quasar spectra corresponding to highly ionized patches of the IGM at z > 6. If correctly interpreted, then the trend in their data suggests that O i abundance may even increase at earlier stages of reionization.

Previous work has proposed exploiting the scattering of UV photons by O i, and the corresponding absorption features in the spectra of quasars: the O i forest (Oh 2002), analogous to the lower redshift H i Lyα forest (e.g., Becker et al. 2006). In the case of H i, another interesting signature from the high-redshift IGM is the 21 cm hyperfine-structure line, which is made detectable by UV pumping by the Lyα background (the so-called Wouthuysen-Field effect; see Field 1958 or Furlanetto et al. 2006 for a recent review). Here we examine whether a similar effect occurs for O i, and demonstrate that there exist O i lines with the required features: the fine-structure lines of the electronic ground state, 44.1, 63.2, and 145.5 μm, can be pumped by 1300 Å photons produced by the first stars or black holes, via the Baic line of O i. We compute the spectral distortion in the CMB created by this effect, and find that it can be as high as y ∼ 10^{-7} if Z_{\odot} at z ∼ 7, just prior to reionization, is ∼10^{-2}Z_{\odot}. Values for the metal abundance of the order of 10^{-3}Z_{\odot} in z ∈ [1, 4] (slightly increasing with redshift) have been observed (Schaye et al. 2003), and since there is less than 1 Gyr between z = 4 and 7, from now on we take Z_{\odot} = 10^{-3}Z_{\odot} as our fiducial value.

This distortion could be detectable with future CMB experiments and opens the possibility of performing tomography of the reionization epoch using this effect. In combination with 21 cm studies, it could yield direct measurements of the abundance and spatial distribution of metals in the high-redshift IGM.4

The basic criteria for a line 0 → 1 of a metal species or their ions to produce an effect analogous to the Wouthuysen-Field pumping of the H i 21 cm line are as follows: (1) abundant metals in the IGM in the required ionization state; (2) the 0 → 1 transition at a frequency suitable for detection, with Einstein coefficients small enough to allow the line to deviate from equilibrium with the CMB; (3) the upper and lower states

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4 Metals will likely be dispersed into the IGM and will not be retained inside the shallow gravitational potential wells of the earliest galaxies (Mac Low & Ferrara 1999). Furthermore, any residual oxygen trapped inside galaxies would be either ionized or in dense, optically thick clumps and would not contribute to the signal.
should be connected via allowed transitions to another state (hereafter called state 2), so that they can be “pumped” in a two-step process; (4) a large background flux at the wavelength $\lambda_{62} \approx 1215 \, \text{Å}$ corresponding to the $0 \leftrightarrow 2$ and $1 \leftrightarrow 2$ transitions. In particular, the last criterion imposes the constraint $\lambda_{62} \lesssim 1215 \, \text{Å}$ on the wavelength of the UV pumping photons before reionization, since neutral H I depletes the background at shorter wavelengths (Haiman et al. 2000).

We selected oxygen for our study because it can be relatively abundant at high redshifts and because of the similarity of its ionization potential to that of hydrogen. The ground state of neutral oxygen is split into the three fine-structure levels of the outermost electrons in the $n = 2$ shell, hereafter denoted as 0, 1a, and 1b. We found that among the electronic states of oxygen, these are the only ones that satisfy all of the criteria above and give rise to photons observable in the CMB frequency band. The states 0–1a and 1a–1b are connected by magnetic dipolar transitions [O I] $^3P_1 \rightarrow ^3P_0$ at 63.2 $\mu$m and $^3P_1 \rightarrow ^3P_2$ at 145.5 $\mu$m, respectively, and the states 0–1b are connected by an electric quadrupolar transition $^3P_1 \rightarrow ^1P_1$ at 44.1 $\mu$m.

We consider only lines involving the 0 state $^3P_0$ as the lower level for the transition, since the CMB ambient field is practically unable to populate the $^3P_0$ state and the 145.5 $\mu$m line will be suppressed. Since these transitions are forbidden, the spontaneous-emission Einstein coefficients ($A_{44.1 \mu m} = 1.34 \times 10^{-10}$, $A_{63.2 \mu m} = 8.91 \times 10^{-5}$, $A_{145.5 \mu m} = 1.75 \times 10^{-5} \, s^{-1}$) are much smaller than the typical values for electric dipole transitions ($\lesssim 10^8 \, s^{-1}$), a property shared by the hydrogen 21 cm line with $A_{21} = 2.85 \times 10^{-35} \, s^{-1}$.

The states 0 and 1a, 1b are connected to the excited electronic state $^3S_i$ in the $n = 3$ shell (hereafter denoted by 2) by means of the absorption of an O i Ba I photon with wavelength $\lambda_{20} \approx \lambda_{12} \approx 1300 \, \text{Å}$. A schematic level diagram is shown in Figure 1. In the absence of a UV field, O i is in thermal equilibrium with the CMB and, as shown in Basu et al. (2004), resonant scattering is more important than collisionally induced emission, except at extremely large overdensities. For this transition, we obtain that the collisions become important at overdensities $\approx 10^5$. However, if the first stars or black holes generated a UV background at 1300 $\, \text{Å}$, then the relative populations of the fine-structure states 0 and 1 are modified by the two-step “pumping” transitions $0 \rightarrow 2 \rightarrow 1$ and $1 \rightarrow 2 \rightarrow 0$.

For simplicity we start by considering only one fine-structure transition and address the combined effect later. In what follows we use the indices $i, j$ to denote the two levels in the fundamental state, with $i$ referring to the lowest one. For example, for the 63.2 $\mu$m transition ($i, j$) corresponds to (0, 1a) (see Fig. 1). The steady state solution for the level population reads

$$n_i = \frac{P_{ij}^{\text{UV}} + B_i I_j}{P_{ii}^{\text{UV}} + B_i I_j + A_i} \approx \frac{g_i}{g_j} \exp \left( -T_{* \leftrightarrow j} \right). \quad (1)$$

This equation defines the spin temperature $T_{* \leftrightarrow j}$. Here $T_{* \leftrightarrow j}$ is the equivalent temperature of the $i \leftrightarrow j$ transition, $T_{* \leftrightarrow j} \equiv h v_{* \leftrightarrow j} / k_B$, $k_B = 231(63.2 \mu m / \lambda_{62}) \, \text{K}$, with $k_B$ the Boltzmann constant; $A_i$, $B_j$, and $B_i$ are the Einstein coefficients for spontaneous emission, induced emission and absorption, respectively; $P_{ij}^{\text{UV}}$ and $P_{ii}^{\text{UV}}$ denote the UV de-excitation and excitation rates; $I_j$ denotes the specific intensity at the resonant frequency of the $i \leftrightarrow j$ transition; and $g_i = 3$, $g_{1a} = 1$, and $g_0 = 5$ are the degeneracy factors. It is useful to define the UV color temperature

$$T_{\text{UV}} \equiv \frac{T_*}{\alpha s} \frac{1}{-\partial \log n_i / \partial v_{r j}} \frac{1}{\nu_{r j}} = \frac{T_{2j}}{3 + \alpha s}, \quad (5)$$

where $n_i \equiv I_i / \nu_i$ is proportional to the number of photons with

![Schematic representation of the transitions of neutral oxygen considered here. Note the analogy with the 21 cm transition of H i. In the 21 cm transition the relevant line corresponds to a hyperfine transition, while for O i it corresponds to a fine-structure transition.](http://physics.nist.gov/PhysRefData/ASD/lines_form.html)
frequency $v$, and $\alpha_s = -d \log I_s / d \log v$ is the logarithmic slope of the background spectrum near the O I $\Delta^2$ line. We have assumed that $\delta \log n_i / \delta v|_{v_2} \approx \delta \log n_i / \delta v|_{v_3}$. For a different approach, see Chuzhoy & Shapiro (2006). If $\delta \log n_i / \delta v|_{v_2}$ is small and negative then the pumping mechanism will be more effective in the transition $i \rightarrow j$ than in $j \rightarrow i$, and as a result the level $i$ will be relatively depopulated. In particular, the $j \rightarrow i$ photons will be seen in emission if $T_{\text{UV}} > T_{\text{CMB}}$, which will generally be the case since $T_z \sim 10^4 K \gg T_{\text{CMB}}$.

The amplitude and shape of the UV photon field at 1300 Å at the beginning of reionization is uncertain. Unlike at the H i Ly$\alpha$ frequency of 1215 Å, however, the high-$z$ IGM should be optically thin at 1300 Å (see discussions of the shape of the soft UV background in Haiman et al. 1996, 2000). Therefore, the relevant background at redshift $z$ should reflect the intrinsic spectrum of the dominant sources over the $\approx 27\%$ redshift range $(1 + z) < (1 + z_{\text{source}}) < (1 + z)_{\text{H i Ly}\alpha} = 1.27(1 + z)^6$. Over the $0.2\%$ fractional difference between $v_2$ and $v_3$, we then expect a relative decrement of $n_i$ of $0.2\%(3 + \alpha_s)$ throughout $v_3$, or a decrement of order $1\%$ for sources with $\alpha_s \sim 2$. For our calculations, we adopted a fiducial choice of $\sim 1\%$, but in practice, our results are insensitive to this value (see below).

Given the specific intensity $I_s$, the steady state solution for the level population provides the following expression for the spin temperature $T_{s,j}$:

$$
T_{s,j} = T_{s,i} \left( \frac{1 + (A_j / P_{jU})|1 + (I_s c^2/2hv)|_{v_j}}{\exp(-T_{s,j} / T_{\text{UV}}) + (A_j / P_{jU})(I_s c^2/2hv)|_{v_j}} \right).
$$

If at a given redshift $z$, the presence of dust can be neglected, $I_s$ at $v_j$ is given by the CMB, $I_i = B_j(T_{\text{CMB}}(z_{\text{source}}))$. In the limit of $A_j \gg P_{jU}$, in equation (6) we have $T_{s,j} \rightarrow T_{\text{CMB}}$, whereas if $A_j \ll P_{jU}$ then $T_{s,j} \rightarrow T_{\text{UV}}$.

As long as the slope of the background at 1300 Å is such that $\alpha_s \sim 1$, equation (5) implies that $T_{\text{UV}} > T_{s,j} > T_{\text{CMB}}(z)$, so that $T_{s,j}$ must be bracketed between $T_{\text{CMB}}(z)$ and $T_{\text{UV}}$. In the limit of $T_{s,j} \ll T_{\text{UV}}$ [and thus $T_{s,j} / T_{\text{UV}} \approx 1$] and $A_j \gg P_{jU}$ (both of these conditions are satisfied for the 63.2 μm line), the departure of $T_{s,j}$ from $T_{\text{CMB}}$ becomes

$$
\frac{T_{s,j} - T_{\text{CMB}}}{T_{\text{CMB}}} \approx T_{\text{CMB}} \frac{g_j A_j}{g_i A_i} \sum A_{2m} \frac{2h\nu_p}{c^2 I_s} \frac{I_s c^2}{2hv}|_{v_j},
$$

i.e., it depends linearly on the UV flux at 1300 Å, and the dependence on $T_{\text{UV}}$ is negligible.

The solid lines in Figure 2 show the deviation of $T_{s,j}$ with respect to $T_{\text{CMB}}$ as a function of the UV flux for $z_s = 10$ (thin line) and $z_s = 7$ (thick line) for the case of the 63.2 μm (0 → 1a) line. While this relative deviation is small ($\sim 10^{-3}$ to $\sim 10^{-4}$), it nevertheless modifies the populations of levels 0 and 1.

The distortion in the CMB spectrum can be parameterized by the $y$-parameter, $y = \Delta T / T_{\text{CMB}}$, where $\Delta T$ is the deviation in surface brightness from the Planck spectrum with the unmodified CMB temperature. Before computing the distortion using the spin temperature above, it is useful to obtain an order-of-magnitude estimate. Because the optical depth of the IGM for the UV photons in our case is small (we find $\tau_{20} = 7.3 \times 10^{-2}$ at redshift 10 for $Z/Z_\odot = 10^{-5}$), multiple scatterings will be rare. (Note that this is different from the case of the H i 21 cm line, where the Ly$\alpha$ photons responsible for the pumping have a large optical depth and scatter multiple times.) In this case, roughly a fraction $\tau_{20}$ of every 1300 Å photon produced by stars will scatter off an O i atom and produce an “excess” $v_j$ photon. Just prior to reionization, assuming that a few UV photons have been produced per H atom (corresponding to a background flux of $J = a \times 10^{-21}$ ergs $^{-1}$ cm$^{-2}$ s$^{-1}$ Hz$^{-1}$), the distortion should be roughly $y \sim f_{\lambda} \tau_{20} \sim 10^{-2}$, where $\eta \times 6 \times 10^{-10}$ is the baryon-to-photon ratio and $f_{\lambda}$ represents the fraction of CMB photon in the frequency band corresponding to the redshift range $\Delta z$.

To compute the distortion of the CMB at the redshifted $v_j$ frequency more precisely, we use the radiative transfer equation $dI / ds = h\nu \Psi(\nu) n_i (A_s + B_s I_s) - n_i B_s I_s / (4\pi)$, with $ds$ the cosmological line element along the line of sight. Since the line profile $\Psi(\nu)$ is narrow, we have ignored the effect of cosmological expansion. For $Z_{\odot}/Z_\odot = 10^5$, we find the optical depth for the 0 → 1a and 0 → 1b transitions

$$
\tau_{20} = \frac{\alpha_s}{8\pi \nu_0 H(z_0)} \frac{g_i}{g_j} \left[ 1 - \exp(-T_{s,0}/T_{s,0}) \right] n_{O_i}(z_s)
$$

to be very small ($\tau_{1a} \sim 2.1 \times 10^{-7}$, $\tau_{1b} \sim 3 \times 10^{-15}$). In this equation we have approximated the line profile function $\Psi(\nu)$ by a Dirac delta, and $\chi^2$ is the fraction of oxygen atoms in the $2^3P$ level to the ground level ($\chi = 1$ to a good approximation). Assuming a constant UV background (justified by the fact that $\tau_{20} \ll 1$), the net change to the CMB due to the
presence of O i can be written as an integral along the line of sight of the emissivity, resulting in

\[ \Delta I^0(\nu) = \frac{h \nu_0 \ e}{4 \pi \ H(\nu_0) \ v_0} \frac{A_0}{n_0} \ g_\nu \ \exp \left( -\frac{T_\nu}{T_{\nu,0}} \right) \ \chi(z_i) \ \frac{1 - \exp \left( \frac{T_\nu}{T_{\nu,0}} - 1 \right)}{2 \ h^2 \ \nu^2 (c^2) \ T_{\nu,0}}. \tag{9} \]

The corresponding CMB distortion at the observed frequency \( \nu = \nu_0/(1 + z_i) \) is given by \( \Delta I^0/\mathcal{B}(\nu_{\text{CMB}}(z_i)) \). In our case \( \tau_0 \ll 1 \), and the distortion parameter can be written in the simple form \( y = \Delta I^0/\mathcal{B}(\nu_{\text{CMB}}(z_i)) \). We find \( \mathcal{B}(\nu_{\text{CMB}}(z_i)) \) and the distortion parameter can be written in the simple form \( y = \frac{T_{\nu,0}}{T_{\nu,0} - 1} \), with \( \tau_0 \ll 1 \).

\[ y = \tau_{63.2} \frac{T_{63.2,0}}{T_{63.2,0} - 1}. \tag{10} \]

In this case, the distortion parameter \( y \) is simply the relative deviation of \( T_{63.2,0} \) with respect to \( T_{\text{CMB}} \) multiplied by the optical depth times the ratio \( T_{63.2,0}/T_{63.2,0} \sim 1 \).

The dashed lines in Figure 2 show the amplitude of the distortion introduced by the O i \( 63.2 \mu \text{m} \) transition at \( z_i = 7 \) (thick line) and 10 (thin line) as a function of the UV background intensity, over a range expected to be relevant for the epoch just prior to reionization. Note that apart from the \( T_{63.2,0}/T_{63.2,0} \) factor, equation (10) is identical to that found for the H i \( 21 \text{ cm} \) spin temperature. Since in our case for \( \tau_{21} \), the relative deviations of \( T_{63.2,0} \) with respect to \( T_{\text{CMB}} \) are typically \( 10^{-3} \) smaller than in the H i \( 21 \text{ cm} \) scenario, and since \( \tau_{10} \sim 10^{-4} \), our \( y \)-distortion is \( \sim 10^{-3} \) smaller than in the \( 21 \text{ cm} \) case. For the 44.1 \( \mu \text{m} \) \( (0 \rightarrow 1 \text{ b}) \) transition, the amplitudes of \( y \) are a factor \( 5 \) larger, but the relevant frequencies are more contaminated by dust and thus more difficult to detect, as we discuss next.

Our basic result is that the O i \( 63.2 \mu \text{m} \) and \( 44.1 \mu \text{m} \) transition could be seen as a deviation in the present-day CMB blackbody spectrum of the order of up to \( 10^{-8} \) at around 160–500 GHz (481 GHz corresponds to \( z = 10 \) and 160 GHz to \( z = 30 \) for the \( 63.2 \mu \text{m} \) transition).

The FIRAS experiment has already obtained constraints on the deviation of the CMB spectrum from a blackbody. We find that in the range of frequencies corresponding to \( 10 < z < 20 \) for the 63.2 \( \mu \text{m} \) line, the FIRAS data (Fixsen et al. 1996) constrain \( y < 10^{-5} \) at the 1 \( \sigma \) level (4 \( \times 10^{-5} \) at the 3 \( \sigma \) level). Considering the expected background UV flux at these redshifts, we obtain a FIRAS constraint of 5 (40) \( Z_\odot \) at \( z_i > 10 \). Although this constraint is far bigger than existing measurements at \( 3 \leq z \leq 5 \) (e.g., Schaye et al. 2003; Aguirre et al. 2004), it is the first direct constraint on the \( Z_\odot \) of the IGM in the universe at \( z \approx 10 \). Since \( y \) scales linearly with \( Z_\odot \), by comparing different, accurately calibrated Planck HFI channels, constraints of \( y < 5 \times 10^{-8} \) could be imposed. An experiment able to reduce the FIRAS \( y \) uncertainty (e.g., Fixsen & Mather 2002) by 2–3 orders of magnitude could impose interesting constraints.

The main limitation to the measurement is foreground dust emission from the Galaxy and from IR galaxies; however, high Galactic latitude patches of the sky and observations at higher frequencies (to remove the IR galaxies) could be used for this purpose. Of course, there could be other cosmological effects (such as decay of particles; see Fixsen & Mather 2002 for a discussion) producing distortion at the feeble \( y \sim 10^{-8} \) level. It remains to be seen whether the O i distortion can be disentangled from these. One further consideration is that clustering of the sources will make it more easily detectable. The signal should trace the clustering properties of the (enriched) fossil H ii regions during reionization and should dominate over the primary CMB angular power spectrum in the damping tail, showing a similar angular pattern to that of the Ostriker-Vishniac effect. In this case the spectral dependence will be different, since this signal is restricted to frequencies probing the O i \( 63.2 \mu \text{m} \) transition at redshifts where \( Z_\odot \) and the UV background are not negligible (C. Hernández-Monteagudo et al. 2007, in preparation). Our technique complements future experiments that will detect the H \( 21 \text{ cm} \) hyperfine transition in absorption because it is sensitive to different systematics and operates at different wavelengths. This would be highly valuable, since H \( 21 \text{ cm} \) + O i measurements in combination can probe the spatial distribution of metallicity directly.

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