A NEW CALCULATION OF THE RECOMBINATION EPOCH

S. Seager\textsuperscript{a} D. D. Sasselov\textsuperscript{b} D. Scott\textsuperscript{c}

\textsuperscript{a}Astronomy Department, Harvard University, 60 Garden Street, Cambridge, MA 02138
\textsuperscript{b}Department of Physics & Astronomy, University of British Columbia, Vancouver, BC, V6T 1Z1

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ABSTRACT

We have recently revisited the calculation of the recombination epoch of the early Universe by making as few approximations as possible and trying to retain full accuracy (Seager, Sasselov, & Scott 1999, hereafter Paper I). We were motivated by the potential to measure (with the MAP and Planck satellites) CMB anisotropies at the roughly 1\% level over a wide range of angular scales, and indications (Hu et al. 1995, hereafter HSSW) that the existing solution for hydrogen and helium recombination has uncertainties at that level. Indeed, we uncovered a number of minor improvements, as well as two more major effects which change the ionization history in a significant way.

Detailed understanding of the recombination process is crucial for modeling the power spectrum of CMB anisotropies. Since the seminal work of the late 1960s (Peebles 1968, Zel’dovich et al. 1968), several refinements have been introduced (see discussion in HSSW and Paper I), but little has changed. Modern codes for evolving the ionization fraction \( x_e \) at a level of 10\% smaller for redshifts \( z < 800 \), due to non-equilibrium processes in the excited states of H. Secondly, the H I recombination is much slower than previously thought, and is delayed until just before H recombines. We describe the physics behind this new result and present a simple way to reproduce our calculation. This should enable fast computation of the ionization history (and quantities such as the power spectrum of CMB anisotropies which depend on it) for arbitrary cosmologies, without the need to consider the hundreds of atomic levels used in our complete model.

\textit{Subject headings:} cosmology: theory — atomic processes — early universe — cosmic microwave background

1. INTRODUCTION

We have recently revisited the calculation of the recombination epoch of the early Universe by making as few approximations as possible and trying to retain full accuracy (Seager, Sasselov, & Scott 1999, hereafter Paper I). We were motivated by the potential to measure (with the MAP and Planck satellites) CMB anisotropies at the roughly 1\% level over a wide range of angular scales, and indications (Hu et al. 1995, hereafter HSSW) that the existing solution for hydrogen and helium recombination has uncertainties at that level. Indeed, we uncovered a number of minor improvements, as well as two more major effects which change the ionization history in a significant way.

Detailed understanding of the recombination process is crucial for modeling the power spectrum of CMB anisotropies. Since the seminal work of the late 1960s (Peebles 1968, Zel’dovich et al. 1968), several refinements have been introduced (see discussion in HSSW and Paper I), but little has changed. Modern codes for evolving the ionization fraction \( x_e = n_e/n_H \) (where \( n_e \) is the number density of electrons and \( n_H \) is the total number density of H nuclei) have been based almost entirely on the single differential equation introduced 30 years ago, with a more accurate recombination coefficient, but no other basic improvement.

With today’s computing power, there is not the necessity for making sweeping approximations that existed 30 years ago. We believe our work represents the most accurate picture to date of how exactly the Universe as a whole became neutral. In this Letter we summarize what is new in the physics involved and present an approximate treatment of our set of equations which accurately reproduces our complete calculation. We discuss in detail the physical basis for each approximation and pay attention to the limits of validity. The paper is supplemented by a computer code (\texttt{recfast}) which can be used to do the calculation, and in conjunction with, e.g. \texttt{cmbfast} by Zaldarriaga, Spergel & Seljak (1997), to compute accurate CMB power spectra for different cosmologies.

2. HOW THE UNIVERSE BECAME NEUTRAL

2.1. Our Multi-level Calculation

In the canonical Hot Big Bang picture, the recombination epoch is when the Universe became cool enough for protons to capture electrons and form neutral hydrogen. This recombination process was not instantaneous, because the electrons, captured into different atomic energy levels, could not cascade instantaneously down to the ground state. The electrons were impeded because of fast reionizations out of excited states due to the huge reservoir of low energy photons, and because of the high optical depth of the Lyman lines and continuum transitions to ground state. Any Lyman line or continuum transition to the ground state emitted a photon with energy where there were few blackbody photons, which immediately photoexcited or photoionized a neighboring atom in the ground state. Atoms reached the ground state through either cosmological redshifting of the Ly\( \alpha \) line photons, or by the 2s–1s two photon process. Because these rates from \( \text{n=2} \) to the ground state were much slower than the net recombination rate to \( \text{n=2} \), a “bottleneck” occurred which slowed down the entire recombination process. The Universe expanded and cooled faster than recombination could have been completed, and a small fraction of free electrons and protons remained. This fraction, during and after recombination, affects the CMB anisotropies through the precise shape of the thickness of the photon last scattering surface (i.e. the visibility function).

The ‘standard’ methodology considers an ‘effective 3-level atom’ with a ground state, first excited state (\( \text{n=2} \)) and continuum, with the states \( \text{n} \geq \text{2} \) represented by a recombination coefficient. A single ordinary differential equation can then be derived to describe the ionization fraction, equation (1) (See Peebles, 1968, 1993). Many
assumptions go into this derivation, including: that H excited states are in equilibrium with the radiation; that stimulated deexcitation is negligible for the Lyα transition; that a simple recombination coefficient can be used; that every net recombination results in a ground state ionized H; that the Lyα redshifting can be dealt with using a simple escape probability; that collisional processes are negligible; and that He can be ignored.

Our new methodology, made possible with modern computing power, is to calculate recombination with as few approximations as possible. Instead of evolving a single ODE for \(dx_e/dt\) for H recombination, we evolve one ODE for each of 300 atomic energy level populations, as well as one for electrons and one for the matter temperature. With this level-by-level treatment, we include thousands of bound-bound transitions which correctly couple the ODEs, and we calculate recombination to each atomic level as it evolves with redshift which eliminates the need for an effective recombination coefficient (\(\alpha\) in §3). We also included other effects (which turned out to be negligible), such as collisional transitions, feedback of distortions to the radiation field, complete heating and cooling terms, and H chemistry. See Paper I for full details on this method. Our new method tests the approximations used in deriving the standard ODE, and we find all of them to be valid, except for the equilibrium assumption. The causes and consequences of this are discussed in §2.2.1, and the effect can be approximated using the single ODE approach, with a small modification that artificially speeds up the recombination at low \(z\), as discussed in §1.

With larger ionization potentials, He I and He II recombined before H. He II recombination shows no deviation from previous calculations, in that we find only small differences compared with Saha equilibrium. However, He I recombination is important for the CMB anisotropies (HSSW), and to some extent for the chemistry in the early Universe (Stancil et al. 1999), and requires closer scrutiny. Our code evolves He I and He II in the same level-by-level method describe above, and simultaneously with H. Previous calculations for He I used the Saha equilibrium method (e.g. HSSW) or an effective 3-level method (Matsuda, Sato & Takeda 1971). We find that the excited states of He I remain in equilibrium with the radiation (unlike H), but that accurate treatment of He I results in a much delayed recombination. This can also be reproduced using a simple ODE for He I.

2.2. What is New in the Physics

2.2.1. Hydrogen

Neutral H production is slightly faster when using our multi-level calculation, compared to the standard calculation (updated with the most recent parameters (HSSW)), as shown in Figure 2.2.1.

For the standard equilibrium case, the net bound-bound rates are zero, and this is an implicit assumption in deriving equation [1]. We find that at \(z \approx 10^3\), the net bound-bound rates become different from zero, because at low temperatures, the cool blackbody radiation field means there are few photons for photoexcitation of high energy transitions (e.g. 70–10, 50–4 etc.). In this case spontaneous deexcitation dominates, causing a faster downward cascade to the \(n=2\) state. In other words, once an electron is captured to, say, \(n=70\), it can cascade down to the \(n=2\) state faster than in the equilibrium case, because few photons are around to photoexcite it. In addition, the faster downward cascade rate is faster than the photoionization rate from the upper state, and one might view this as radiative decay stealing some of the population “flux” from photoionization. Both the faster downward cascade and the lower photoionization rate contribute to the faster net recombination rate.

![Fig. 1: Multi-level hydrogen recombination for the standard CDM parameters \(\Omega_m = 1.0, \Omega_B = 0.05, H_0 = 50, Y_p = 0.24, T_0 = 2.728K\). The two lines are the complete calculation of Paper I (dotted) and the standard (effective 3-level atom) calculation (dashed).](image_url)

An imbalance develops as the background radiation continues to cool while the entire Lyman series remains optically thick (the “bottleneck” gets worse). A Boltzmann distribution relative to \(n=2\) is no longer sustainable — the excited states become progressively overpopulated. (Note that this is not a population inversion.) The radiation field is cool, but strong, and able to keep neighbouring states well coupled, as well as to hold the highest Rydberg states in equilibrium with each other. However, in comparison with the standard equilibrium capture-cascade calculation for \(\alpha\), this unusual situation leads us to higher effective recombination rates to the majority of excited states, without increasing photoionization proportionally. This results in a higher net rate of production of neutral hydrogen atoms.

Because the net effect of our new H calculation is a faster recombination (a lower freeze out ionization fraction), our results can be reproduced by artificially speeding up recombination in the standard calculation, simply by multiplying the recombination and ionization coefficient by a ‘fudge factor’ \(F\).

2.2.2. Helium

Our new multi-level calculation shows a significantly delayed He I recombination compared to previous calculations. In fact, for our low \(\Omega_m\) models He I recombination is still finishing at the very beginning of H recombination. Figure 2.2.2 shows the ionization fraction \(x_e\) through He II, He I and H recombination, plotted against the standard H calculation and He II and He I recombination calculated...
using the Saha ionization equilibrium equation.

Fig. 2: Helium and hydrogen recombination for the standard CDM parameters with $Y_p = 0.24$ and $T_0 = 2.728$ K. The first step from right to left is recombination of He III to He II, the second step is He II to He I. The dashed line is our new He I calculation, while the dotted line is the He Saha equilibrium recombination and the H standard calculation.

The recombination of He I is slow for the same reasons that H recombination is, namely because of the optically thick $n^3p - n^1s$ transitions which make cascades to the ground state slow, and the exclusion of recombinations to the ground state. In other words He I follows a Case B recombination with an inhibition factor. Because the "bottleneck" at $n=2$ largely controls recombination, it is not surprising that He I and H recombination occur at a similar redshift; the ionization energy of $n=2$ is similar to the ground state. In other words He I slow, and the exclusion of recombinations.

The physics of He I recombination is different than that for H recombination because of its different atomic structure. More specifically, the high excited states of He I are much more strongly packed towards the continuum compared to those of H; the energy difference between the 3p levels and the continuum is 1.6 eV for He I versus 1.5 eV for H, compared to 24.6 eV versus 13.6 eV for the ground state. Because of this, the radiation field has a stronger effect on the excited states of He I than those of H. This has 3 main consequences: 1) The strong radiation field during He I recombination keeps the ratio of photoionization rate to downward cascade rate higher than the H case, resulting in a slower recombination than H. 2) The strong radiation field also causes the triplet states (e.g. $n^3p - n^1s$) to be virtually unpopulated. The triplets have only forbidden (i.e. very slow) transitions with the singlets, and a metastable "ground state" 4.77 eV from the continuum. 3) The radiation field is strong enough that the excited states remain in equilibrium with the radiation throughout recombination.

There is one possibility to speed up the slow He I recombination. It is the existence of some neutral H, which could ‘steal’ He I resonance line photons, invalidate the effective Case B by removing the “bottleneck” at $n=2$, and make it a Saha equilibrium recombination instead. However, our detailed calculation shows that the rate for this process never comes close to being significant.

Because He I recombination simply follows a Case B recombination and unlike for H the excited singlet states remain in equilibrium throughout recombination, it can be reproduced using the effective 3-level single ODE (shown below). Because the triplet excited states remain unpopulated during recombination, the effective 3-level atom is the ground state 1’s, the first singlet excited state, and the continuum.

3. THE APPROXIMATE SET OF EQUATIONS

Here we present a set of equations which allow a simple way to reproduce our new recombination results from the multi-level code. Though approximate, the set provided below includes more of the recombination physics than the ‘standard’ calculation, and reproduces approximately (via parametrizations) the departures from equilibrium in H, and the slow He I recombination found in Paper I.

However, a word of caution is necessary – the set of equations below have a range of validity which corresponds roughly to the choice of typical cosmologies discussed in Paper I. Attempts to calculate recombination in more extreme cosmologies, or with the addition of extra physics, will probably require evolution of the full set of equations of the multi-level code. In addition, our approximations here are designed for optimal use with the CMB anisotropies, and do not fit as well the range below $z \sim 300$, where molecular formation becomes important. Therefore detailed study of the chemistry in the early universe will probably also require evolution of the full set of equations of the multi-level code.

The approximate set of equations below — two ODEs for the ionization fractions of H and He I, and an equation for the matter temperature — should be solved simultaneously. We recommend leaving out He II recombination entirely, since it has no effect on the power spectrum of CMB anisotropies. Otherwise Saha equilibrium is an adequate approximation. The two ODEs derive from consideration of detailed balance in the effective 3-level atoms of H and He I (see Peebles, 1968, 1993). The total recombination coefficients in each case have been parametrized to reproduce our multi-level results. The equation of the total rate of change of the matter temperature is a truncated version of Paper I eq. (69), including adiabatic and Compton cooling terms. The set is as follows:

$$\frac{d\alpha_{HeI}}{dz} = \left( x_{HeI} x_{n^1s} \alpha_{HeI} - \beta_{HeI}(1 - x_{HeI}) e^{-h\nu_{HeI}/kT_M} \right) \times \frac{1 + K_{HeI} (1 - x_{HeI})}{H(z)(1 + z)(1 + K_{HeI}(1 + \alpha_{HeI})(1 - x_{HeI}))},$$

$$\frac{d\alpha_{HeII}}{dz} = \left( x_{HeII} x_{n^1s} \alpha_{HeII} - \beta_{HeII}(1 - x_{HeII}) e^{-h\nu_{HeII}/kT_M} \right) \times \frac{1 + K_{HeII} (1 - x_{HeII})}{H(z)(1 + z)(1 + K_{HeII}(1 + \alpha_{HeII})(1 - x_{HeII}))},$$

$$\alpha_{HeI} = F 10^{-19} \frac{a_{I}}{1 + c T^3} \text{m}^3 \text{s}^{-1},$$

$$\alpha_{HeII} = q \left[ \sqrt{\frac{T_M}{T_2}} \left( 1 + \sqrt{\frac{T_M}{T_2}} \right)^{-p} \left( 1 + \sqrt{\frac{T_M}{T_1}} \right)^{1+p} \right]^{-1} \text{m}^3 \text{s}^{-1},$$

where $T_M$, $T_1$, and $T_2$ are the temperatures of the microwave background, He II, and H I, respectively, and $q$ is a parameter that accounts for the effect of Compton cooling. The recombination coefficients $\beta_{HeI}$ and $\beta_{HeII}$ are obtained from the Saha equation, while the term $\alpha_{HeI}$ and $\alpha_{HeII}$ represent the recombination coefficients for the He I and He II cases, respectively.
\[
\frac{dT_M}{dz} = \frac{8\pi T_R^4}{3H(z)(1 + z)m_e c} x_e \left( \frac{T_M - T_R}{1 + f_{He} + x_e} + \frac{2T_M}{(1 + z)} \right)
\]  

(5)

Equation (5) is for the matter temperature, which we recommend to use in the entire calculation above, due to the small but important effect resulting from the difference between \( T_M \) and \( T_R \) at low redshift. Below we list all constants and parameters which appear in the above equations.

The constants are Boltzmann’s constant \( k \), Planck’s constant \( h \), the speed of light \( c \), Thomson scattering cross section \( \sigma_T \), the electron mass \( m_e \), and the radiation constant \( a_R \). The three independent variables are proton fraction \( x_p = n_p/n_H \), singly ionized helium fraction \( x_{HeI} = n_{HeI}/n_H \), and matter temperature \( T_M \). The dependent variable is the electron fraction \( x_e = n_e/n_H = x_p + x_{HeI} \). Here \( n \) refers to number density, and \( n_H \) is the total hydrogen number density.

Turning to the atomic data, the H Ly\( \alpha \) rest wavelength is \( \lambda_{H\alpha} = 121.5682 \, \text{nm} \). The H 2\( s\)–1\( s \) frequency \( \nu_{H\alpha} = c/\lambda_{H\alpha} \), is close enough to Ly\( \alpha \) that the same averaged wavelength value can be used. The He I 2\( p\)–1\( s \) wavelength is \( \lambda_{HeI} = 58.4334 \, \text{nm} \). Note that the He I 2\( s\)–1\( s \) frequency \( \nu_{HeI} \) is \( c/\lambda_{HeI} = 60.1404 \, \text{nm} \). Unlike for H, the separation of He I 2\( p\) and 2\( s\) is large enough that \( \lambda_{HeI} > \lambda_{H\alpha} \) must be distinguished, hence the extra exponential term in equation (2) over equation (1), with \( \nu_{HeI} = \nu_{HeI} + \nu_{HeII} \). (where we define this last notation to save space). The H 2\( s\)–1\( s \) two photon rate is \( \Lambda_{H\alpha} = 8.22458 \times 10^{-1} \) (Goldman, 1989), while the He I 2\( s\)–1\( s \) two photon rate is \( \Lambda_{HeI} = 5.31 \times 10^{-1} \) (Drake et al., 1969).

Further, \( \alpha_{He} \) is the Case B recombination coefficient for He, from Hummer (1994), and fitted by Péquignot et al. (1991), with \( a = 4.309 \), \( b = -0.6166 \), \( c = 0.6703 \), \( d = 0.5300 \), and \( t = T_M/10^4 \, \text{K} \). The factor \( F \) is 1.14, and allows equation (6) to agree with our multi-level calculation by speeding up recombination. Note that it also enters into the coefficient \( \beta \) via \( \alpha \) as described below. \( \alpha_{He} \) is the Case B He I recombination coefficient for singlets, from Hummer and Storey (1998). The parameters are \( q = 10^{-10.744} \), \( p = 0.711 \), \( T_1 = 10^5 \, \text{K} \), and \( T_2 \) fixed arbitrarily at 3 K. This fit is good to about 0.1% over the relevant temperature range (4,000–10,000 K), and still fairly accurate over a much wider range of temperatures. The \( \beta \) are photoionization coefficients and are calculated from the recombination coefficients by: \( \beta = \alpha(2\pi m_e k T_M/k^3)^3/2 \exp(-h\nu_2/kT_M) \). Here \( \nu_2 \) and \( \alpha \) are different for H and He I. Note that \( T_M \) and \( \nu_2 \) are used here, and that incorrectly using \( T_R \) or \( \nu_2 \) will cause a small but important difference for high baryon models.

The cosmological parameters are the redshift \( z \), Hubble factor \( H(z) \), the cosmological redshifting of H Ly\( \alpha \) photons \( K_H \equiv \lambda_{H\alpha}^2 / (8\pi H(z)) \), the cosmological redshifting of He I 2\( p\)–1\( s \) photons \( K_{HeI} \equiv \lambda_{HeI}^2 / (8\pi H(z)) \), and the radiation temperature \( T_R = T_0(1 + z) \). The primordial He abundance was taken to be \( Y_p = 0.24 \) by mass (Schramm & Turner, 1998), and the present-day CMB temperature \( T_0 \) to be 2.728 K (the central value determined by the FIRAS experiment, Fixsen et al. 1996).

A word of caution about the numerical computation. The equations are generally stiff, and so there are two approaches which can be taken. One is to use an integrator appropriate for stiff sets of equations, the other is to use Saha equilibrium values of \( x_e \) to carry the integrations through the stiffest regimes (the beginning of each recombination epoch). The former case is not much slower, and certainly will work for arbitrary cosmology. For the latter case some experimentation may be necessary in order to efficiently choose the redshift to start and finish the Saha approximation for particular cosmologies, and then it may be faster.

For He II it is sufficient to use the relevant Saha equation:

\[
\frac{(x_e - 1 - f_{He}) x_e}{1 + f_{He} - x_e} = \frac{(2\pi m_e k T)^{3/2}}{h^3 n_H} e^{-\chi_{HeII}/kT} \tag{6}
\]

For the non-stiff integrator approach, this can be switched on at say \( z > 5,000 \). Then there will be a period when He is all singly ionized, and after say \( z = 3500 \) the Saha equation for He I needs to be switched on:

\[
\frac{(x_e - 1)x_e}{1 + f_{He} - x_e} = \frac{4(2\pi m_e k T)^{3/2}}{h^3 n_H} e^{-\chi_{HeI}/kT}. \tag{7}
\]

This can be used until say 1% of the He I has recombined, at which point the coupled ODEs can be solved using a routine such as dverk (Hull et al., 1976). It is also worth fixing the hydrogen to be fully ionized until some redshift, then using Saha for H to get recombination started. It may also save some integration time if He recombination is switched off once the fraction of neutral He has fallen below some small number.

We found that in fact it was not necessary to evolve the H and He equations simultaneously, at least for cosmologies which we checked in detail. It appears to be sufficient to evolve each separately, even in cases where there is a small overlap in the recombination epochs. However, there is little computational expense in solving the 3 ODEs simultaneously, and so that is what we recommend.

4. CONCLUSION

We have presented the basic physics behind our improved recombination calculation which shows a significantly delayed He I recombination and a 10% lower residual \( x_e \) at freezeout compared to previous calculations. We present a set of equations to reproduce our work, which are modified versions of those previously used because our new, detailed calculation agrees very well with the results of the standard calculation. This underscores the tremendous achievement of Peebles, Zel’dovich and colleagues in so fully understanding cosmic recombination 30 years ago. However, the goal of modern cosmology is to determine the cosmological parameters to an unprecedented level of precision, and in order to do so it is necessary to understand very basic things, like recombination, much more accurately.

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