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Recombination lines in the primordial radiation

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An accurate numerical calculation is made for the intensity and profiles of hydrogen recombination lines of cosmological origin. The dependence of these quantities on parameters of matter in the universe is established: on the hydrogen density and on the total density of all kinds of matter.

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1. We shall consider in this paper the distortions in the primordial background (vestigial) radiation caused by the release of recombination photons as matter cooled and was transformed from a fully ionized into a neutral state during the early stages in the evolution of the universe. Zel'dovich, Kurt, and Syunyaev[1] have examined the dynamics of hydrogen recombination in a hot or big-bang model universe, and have shown that the most powerful distortions that could have arisen in the frequency range corresponding to the Lyman lines would not have survived, because inverse capture of the high-energy photons liberated in this manner would have taken place. The main process ensuring an irreversible transition of electrons to the first level turns out to be two-photon decay of the 2S level.

One of us has pointed out previously[2,3] that distortions exist corresponding to transitions between highly excited levels in the hydrogen atom. It has been shown that these distortions will in fact survive, and their amplitude has been estimated roughly. The argument has been made that an experimental detection of these distorting effects would enable fundamental parameters of the universe to be determined: the hydrogen density and the total density of all types of matter.

We give below an exact numerical calculation of the intensity and profile of the distortions described in these papers.[2,3] The intensity will be found to comprise $\approx 5 \cdot 10^{-6}$ of the primordial background radiation for the case of a transition from the 17th to the 16th level, which corresponds to a present wavelength $\lambda = 30$ cm (it is here assumed that the density of matter is equal to the critical density).

2. Let us consider the kinetics of hydrogen recombination at a temperature $T = 4000°K$ and a density $n = 10^4$ cm^{-3}. Recombination will take place because of the drop in temperature as the universe expands. Energy will be released corresponding to a transition of electrons from the free to the bound state. This energy will appear in the form of superequilibrium recombination photons, that is, photons in excess of the background Planck radiation. The whole recombination process operates in a quasiequilibrium fashion: At any epoch the background radiation remains Planckian because of the isotropy of the expansion and the independence of the red shift on frequency, but the temperature of matter is very close to the radiation temperature because of the Compton effect. Under these conditions a slow rise in the number of neutral atoms will occur against the background of a large number of recombination and ionization events, which serve to maintain the dynamical equilibrium of matter and the background radiation.

The superequilibrium photons released by the irreversible recombination process will interact with matter. One finds that for all photons other than those of the Lyman series, this interaction, during the time span of interest to us, is unimportant. But the Lyman photons will rapidly be absorbed because of the high population of the first level. Upon being absorbed, a Lyman photon emitted in an $i \to 1$ transition (where i is the number of the level) will induce a $1 \to i$ transition, returning the system to its original state; thus we may regard transitions from the first and to the first level as not taking place at all. Ultimately, however, the electron will arrive in the ground state by means of two-photon decay of the 2S level.

3. We turn now to a general formulation of the problem. As will be evident from the considerations above, we should be interested only in irreversible recombination events. In each such event a certain set of photons

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will be released, corresponding to the trajectory with respect to levels that the recombining electron describes as it heads toward the ground state. We shall be interested in the mean number $\varkappa_{ij}$ of photons of a specified frequency (representing the transition from level i to level j) released in a single irreversible recombination event.[2,3] Generally speaking, $\varkappa_{ij}$ will depend on temperature, but as we shall show presently, in the temperature range $4200 > T > 3800°K$ of interest to us, this dependence is very weak ($\approx 1\%$).

By the definition of $\varkappa_{ij}$, the number of superequilibrium photons will be

$$\delta N_{ij}=\varkappa_{ij}\delta N_0,$$

where δN_0 is the number of irreversible recombination events, or, equivalently, the change in the number of free electrons or neutral atoms. Photons released at different epochs and accordingly at different red shifts z will have different frequencies at the present time. Evidently $\Delta\nu/\nu = \Delta z/(1+z)$.

For greater clarity it is convenient to use a differential property of the distortion amplitude: the ratio of δN_{ij} to the number δN_r of photons in the Planck radiation at the same frequency and in the same frequency band. This ratio $K = \delta N_{ij}/\delta N_r$ is given[2,3] by

$$K=\varkappa_{ij}\frac{\lambda_{ij}^2\hbar c}{4kT_0}\omega n_c\frac{dx}{dz}z^3,$$

where λ_{ij} is the laboratory wavelength of the $i \to j$ transition, $\hbar$ is the Planck constant, c is the velocity of light, k is the Boltzmann constant, T_0 is the radiation temperature at $z_0 = 1500$, n_c is the critical density for hydrogen at z_0, $\omega = n_H/n_c$, n_H is the density of hydrogen, z denotes the value of the red shift referred to z_0, $x = n_0/n_H$, and n_0 is the density of neutral hydrogen atoms. Upon substituting numerical values and taking a Hubble constant $H_0 = 75$ km · sec^{-1} · Mpc^{-1} we obtain (for $\lambda_0 = \lambda_{17,16} = 2\cdot10^{-2}$ cm)

$$K=1.27\cdot10^{-4}\varkappa_{ij}\omega\left(\frac{\lambda}{\lambda_0}\right)^2\frac{dx}{dz}z^3.$$

We have therefore to calculate $\varkappa_{ij}$ and $f = z^3(dx/dz)$.

4. Our procedure for evaluating the efficiency factor $\varkappa_{ij}$ — the mean number of photons of frequency ν_{ij} released for each irreversibly recombining electron — is based on a modeling of the motion of the electron with respect to levels. This motion is determined by the matrix W_{ij} of relative transition probabilities from level i to level j. To simplify the calculations we appeal to the fact that looped trajectories — those beginning and ending at the same level — make no contribution to $\varkappa_{ij}$, because each such trajectory will correspond to an inverse one of the same probability, in view of the detailed balancing principle.

The calculation scheme thereby reduces to the following. In a system consisting of discrete levels (beginning with the second), with the transition probabilities between them being specified by the matrix W_{ij}, a certain number of particles will be triggered at initial time which are distributed with respect to levels according to the probabilities $W_{\infty j}$ of recombination on those levels. In the first step these particles will be redistributed over all levels (including the infinite level, which corresponds to the continuum) in accordance with the matrix W_{ij}, which is formally equivalent to multiplying the population vector n_i by the matrix W_{ij}. Particles that become ionized will be excluded from further consideration since they describe loops $\infty \to \ldots \to \infty$. We similarly shall neglect particles arriving on the second level, because their subsequent motion will necessarily terminate on the second level, again leading to a loop: $2 \to \ldots \to 2$. The next step proceeds analogously, and so on. The calculation ends when the number of particles neither becoming ionized nor reaching the ground state becomes sufficiently small. In each step we record the number of photons of frequency ν_{ij} released, namely $n_iW_{ij} - n_jW_{ji}$; we then sum these numbers and divide the sum by the total number of particles reaching the second level. The quantity obtained is the required value of $\varkappa_{ij}$. A description of the matrix W_{ij} used in the calculation is given in Appendix 1.1.

5. The recombination dynamics is determined by the rate at which the superequilibrium Lyman photons are redistributed. As Zel'dovich et al.[1] have shown, the principal mechanism in the redistribution process is two-photon decay of the 2S level. They have also obtained an equation describing the change in the degree of ionization with time. We wish to point out, however,[3] that Zel'dovich et al. neglect the difference in the hydrogen density n_H in the universe from the density n_t ($\Omega = n_t/n_c$) of all types of matter (helium and other possible forms of matter, such as neutrinos, gravitational waves, and black holes). These two densities affect the recombination dynamics differently: Ω determines the expansion rate of the universe, and ω is the total number of recombination events.

With this situation in mind, we rewrite the equation of Zel'dovich et al. in the form

$$\frac{dx}{dz}=A_{2S,1S}H^{-1}\Omega^{-1/2}z^{-5/2}e^{I/4kT_0z}\left[x^2\left(\frac{1-x_0}{x_0^2}\right)-(1-x)\right],$$

where $A_{2S,1S} = 8.2$ sec^{-1} represents the probability of two-photon decay, $H = h\cdot 75$ km · sec^{-1} · Mpc^{-1} is the Hubble constant, $I = 13.6$ eV, and x_0 is given by the Saha formula:

$$\frac{x_0}{1-x_0}=\left(\frac{mkT_0z}{2\pi\hbar^2}\right)^{3/2}\frac{1}{n_H}e^{-I/kT_0z}.$$

6. In many respects the fate of the photons liberated depends on whether they can survive interactions with matter. The chief interaction mechanisms are: broadening by electron collision, free—free and free—bound absorption, and bound—bound absorption followed by reprocessing into other photons. Allowance must be made for the fact that photons released at different times will pass through layers of differing optical thickness. This effect will introduce a further distortion into the line profile. Henceforth all optical depths τ will be taken from the epoch z_1 of release of a given photon.

The broadening by electron collision is expressed by

$$\frac{\Delta\nu}{\nu}=6\cdot10^{-2}\frac{\omega^{1/2}}{h^{1/2}\Omega^{1/4}}\left(\int_0^{z_1}xz\,dz\right)^{1/2}.$$

TABLE I

i	i+1	i+2	i+3	i+4	i+5	i	i+1	i+2	i+3	i+4	i+5
8	20.3	9.06	5.41	3.65	2.65	17	4.68	2.20	1.39	0.98	0.75
9	16.4	7.34	4.42	3.01	2.20	18	4.18	1.97	1.25	0.89	0.67
10	13.3	6.01	3.65	2.51	1.85	19	3.76	1.78	1.13	0.8	0.61
11	11	5.03	3.08	2.13	1.58	20	3.39	1.61	1.02	0.73	0.56
12	9.29	4.27	2.63	1.83	1.36	21	3.08	1.46	0.93	0.66	0.51
13	7.95	3.68	2.28	1.59	1.19	22	2.81	1.34	0.85	0.61	0.47
14	6.87	3.20	1.99	1.40	1.05	23	2.57	1.28	0.78	0.56	0.43
15	6	2.80	1.75	1.23	0.93	24	2.36	1.13	0.72	0.52	0.4
16	5.28	2.48	1.55	1.10	0.83						

TABLE II

$\hbar\Omega^{1/2}$	ω										
	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1
0.45	0.38	0.91									
0.55	0.36	0.87	1.44	2.28							
0.65	0.34	0.83	1.38	1.96	2.56	3.18					
0.75	0.32	0.80	1.33	1.91	2.50	3.10	3.72	4.36			
0.85	0.31	0.77	1.29	1.85	2.43	3.04	3.65	4.28	4.90		
0.95	0.29	0.74	1.25	1.80	2.38	2.97	3.57	4.20	4.81	5.45	6.10
1.05	0.28	0.72	1.23	1.75	2.32	2.90	3.50	4.13	4.73	5.32	6.01
1.15	0.27	0.70	1.20	1.71	2.27	2.84	3.44	4.06	4.66	5.28	5.92
1.25	0.26	0.68	1.17	1.67	2.22	2.79	3.38	3.97	4.58	5.20	5.83
1.35	0.25	0.65	1.15	1.63	2.17	2.73	3.32	3.91	4.51	5.13	5.75
1.45	0.24	0.63	1.12	1.59	2.13	2.68	3.26	3.84	4.44	5.05	5.68
1.55	0.24	0.62	1.10	1.56	2.08	2.63	3.20	3.78	4.37	4.98	5.61

The optical depth for free–free transitions is

$$\tau_{f-f}=4\cdot10^{-3}\frac{\omega^2}{\hbar\Omega^{1/2}}\lambda^2\int_0^{z_1}x^2z^2\,dz;$$

for free–bound transitions,

$$\tau_{f-b}=4\cdot10^{-3}\frac{\omega^2}{\hbar\Omega^{1/2}}\lambda\int_0^{z_1}x^2z^{1/2}\,dz;$$

and for bound–bound transitions, allowing for emergence from the profile because of the expansion of the universe,

$$\tau_{b-b}=10^{-2}x^{-2}\frac{\omega^2}{\hbar\Omega^{1/2}}\lambda,$$

where λ is the present value of the wavelength.

A few words are in order with regard to this last mechanism. Absorption in lines will not of itself annihilate a photon. Such an event will occur only if an inverse transition fails to bring the electron to the same level, or if capture of another photon from the radiation field takes place and the system does not revert to its initial state by a strictly inverse route. In either case, one photon from the external field will disappear and a photon of the combined frequency will be generated. Simple thermodynamical considerations – the condition that entropy grow – imply that such a process should operate in the sense of formation of a photon whose frequency lies as close as possible to the maximum of the Planck distribution.

7. The results of our calculation of $\varkappa_{ij}$ are given in Table I. Values of this efficiency factor are given here for levels i and j differing by a small number. The numbers i and j themselves have been selected within the interval of greatest interest. From Table I we may, in particular, determine the relative intensity of the principal (i – j = 1) and satellite (i – j > 1) lines having approximately the same frequency.

A byproduct of the calculation of $\varkappa_{ij}$ is the value of the transmission coefficient γ_i, representing the probability that an electron from the i-th level will reach the second level. We omit a table of values of γ_i, pointing out only that γ_i decreases rapidly with increasing i, and amounting generally to a few percent for 60-70 levels. In other words, the contribution of the high levels is very slight, so that it is immaterial how many levels we take into account.

Knowing γ_i, we can estimate the intensity of the distortions produced in free–bound transitions. For instance, in the case of transitions $\infty \to 50$-60 (corresponding to the frequency of the 17–16 line), the intensity $\delta N_{\infty,50} \approx 10^{-3}\,\delta N_{17,16}$. We here make use of the fact that the $\infty \to i$ lines, where i > 10, are strongly blurred by the continuity of the free-electron spectrum. For $\infty \to i$ transitions in which i < 10, the lines are narrower. The most intense and narrow line ($\Delta\nu/\nu \approx 0.05$) corresponds to the Balmer jump H_C. For this line we obtain

$$\frac{\delta N_{\infty,2}}{\delta N_2}\approx 10^{-5}$$

at wavelength λ ≈ 0.6 mm. Observation of this line would be advantageous because it is isolated and occurs in a wavelength range where the receiver can have a bandwidth about 500 times as large as $\lambda_{17,16}$.

Table II gives the maximum values of the coefficient f (see Sec. 3) for selected values of ω and Ω. These have

been found by numerical integration of the dynamical equations in Sec. 5.

8. We conclude with a few words about helium. Recombination of the first electron for helium will take place at a red shift z_{He} differing by several percent from $4z_{max}$. This will be the case because the presence of a factor preceding the exponential in the Saha formula, as well as differences in the recombination dynamics due to the relative overabundance of electrons. The helium lines will therefore be shifted relative to the hydrogen lines. They will be about 30 times weaker than the hydrogen lines because, in the first place, helium is about 12 times less abundant than hydrogen by number of particles, while in the second place, strongly broadening ($\Delta\nu/\nu \approx 0.3$) is produced by electron scattering, since the elapsed time from the recombination of helium to the disappearance of the free electrons is very long.

Recombination of the second electron will be ineffective for the same reason. Certain more delicate mechanisms for generating spectral distortions associated with helium will be considered in a future paper.

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APPENDIX 1

In order to calculate the values we need for the efficiency $\varkappa_{ij}$ with which a particular photon is released, we must model the motion of an electron with respect to levels. This motion is described by the matrix of transitions r between levels and transitions e caused by collisions with electrons are possible. Hence the probability A_{ij} of a transition from the i-th to the j-th level will be given[4] by

$$A_{ij} = A_{ij}^{(r)} + A_{ij}^{(e)}, \quad i>j,$$

where

$$\left.\begin{aligned} A_{ij}^{(r)} &= A_0^{(r)} \nu_{ij}^2 \frac{j^2}{i^2} \frac{ji^3 g_{ij}}{(i^2-j^2)^3} (1+N_{ij}), \\ A_{ij}^{(e)} &= A_0^{(e)} \frac{i^3 j g_{ij}}{(i^2-j^2)^3} N_{ij} n_e, \end{aligned}\right\}$$

$$N_{ij} = \left[\exp\frac{2\pi\hbar\nu_{ij}}{kT} - 1\right]^{-1}.$$

Since the ratio of $A_{ij}^{(e)}$ to $A_{ij}^{(r)}$ is proportional to i^6, we can establish a limit ($i \approx 65$) above which there are only collisional transitions, and below, only radiative transitions. Including stimulated processes, the recombination coefficient $\alpha_i = A_{\infty,i}$ is given by

$$A_{\infty,i} = \alpha_i = \alpha_0 \int_{u_i}^{\infty} \frac{du}{u(e^u-1)}; \quad u_i = \frac{\chi_i}{kT}.$$

Correspondingly, the ionization coefficient $\beta_i = A_{i,\infty}$ is

$$\beta_i = \beta_{0i} \frac{1}{i^2} \int_{u_i}^{\infty} \frac{du}{u(e^u-1)}.$$

For direct calculation it is desirable to take as many more levels into account as possible, up to a limit at the continuous spectrum. We have considered a system of 500 levels, but we have made the following simplifications. As already mentioned, beginning at the 60th level the predominant role is played by collisional transitions, which have a strong dependence on $i-j$ and higher probabilities with respect to the ionization probability. Accordingly, an electron will diffuse for a fairly long time in the neighborhood of these levels, producing nearly an equilibrium distribution of populations. All levels above the 70th have therefore been combined into one by averaging the transition probabilities from those levels to lower ones (below the 70th) and back with Boltzmann populations. Check calculations show that the overall result depends little on the details of averaging and the limits. We note that all these calculations have been performed for transition probabilities averaged over the orbital momentum. However, analysis of the manner in which the splitting of the levels with respect to momentum affects the A_{ij} indicates that to a first approximation it may be neglected.

Since the calculation is carried out in steps corresponding to a transition to some particular level rather than in real time, we use the matrix W_{ij} of relative transition probabilities:

$$W_{ij} = \frac{A_{ij}}{\sum_{j=2}^{\infty} A_{ij}}, \quad i=2,3,\ldots,\infty; \quad W_{ii}=0.$$

APPENDIX 2

Mathematically, the efficiency has formally been calculated by the following procedure. We have a transition matrix W_{ij}, where i, j = 2, 3, ..., 71, ∞ (71 represents a unified level, embracing electrons from levels 71 to 500, while the "level" ∞ corresponds to the continuum). We introduce a vector n_i (i = 2, 3, ..., ∞) for the distribution of population with respect to levels. At step 0 we take $n_i^{(0)} = W_{\infty,i}$. At each successive step the electrons are redistributed according to

$$n_j^{(k)} = \sum_{i=3}^{71} n_i^{(k-1)} W_{ij}, \quad j=3,4,\ldots,71;$$

$$n_j^{(k)} = n_j^{(k-1)} + \sum_{i=3}^{71} n_i^{(k-1)} W_{ij}, \quad j=2,\infty.$$

We now compute the number of photons released in the line $i \to j$:

$$P_{ij}^{(k)} = n_i^{(k-1)} W_{ij} - n_j^{(k-1)} W_{ji}, \quad i,j=3,\ldots,71,\infty.$$

The calculation terminates at step $\bar{k}$, when $n_2^{(\bar{k})} + n_\infty^{(\bar{k})} > 0.99$. Afterward we calculate the quantities $P_{ij} = \sum_k P_{ij}^{(k)}$ and set $\varkappa_{ij} = P_{ij}/n_2$. We also compute the transmission coefficient $\gamma_{2,\infty} = n_2(\bar{k})$.

Similar calculations have been performed in the case where the initial population vector $n^{(0)}$ has the form $n_i^{(0)} = 0$ for $i \neq m$, $n_m^{(0)} = 1$; in other words, we consider the fate of the electrons that originally arrived on the m-th level. The efficiency

$\varkappa_{ij}(m)$ has been evaluated for such electrons as well as the transmission coefficient $\gamma_{2,m}$. These data have been used to check the calculations; in addition, they are of independent interest for the asymptotic recombination problem.

A further check has been a calculation of the number of photons in the line $i \to j$ released by electrons that subsequently reach the level α. The purpose of this calculation was to verify that the loops make a zero contribution at the machine level, so to speak. If the matrix A_{ij} was correctly specified, the effect, as anticipated, was found to be zero.

The solution was checked for stabilities against variation of the various parameters. The limit of averaging was varied (instead of the 70th level, the 50th or 90th was taken), and the electron density in the expression for $A_{ij}^{(e)}$ (Appendix 1) was changed by an order of magnitude in either direction. It was found that although the transmission coefficient $\gamma_{2,\infty}$ varies by a factor of 1.3-1.5, the efficiency remains constant to better than 1%..

Calculations have also been performed to correct for the splitting of the second level (since two-photon decay takes place from the 2S but not the 2P level). This splitting also does not influence the results

APPENDIX 3

There is an alternative method for calculating the efficiency $\varkappa_{ij}$, based on a consideration of the balance equation. The balance equations have the form

$$n_i \sum_{j=2}^{\infty} A_{ij} = \sum_{j=2}^{\infty} n_j A_{ji} \quad \text{for} \quad i>2,$$

$$n_2 \sum_{j=3}^{\infty} A_{2j} + J = \sum_{j=3}^{\infty} n_j A_{j2},$$

where n_i denotes the population of the i-th level and J represents a small loss from the second level due to irreversible recombinations.

For a specified loss J, we can determine from these equations the deviation Δn_i of the populations n_i from their equilibrium values; we then find $\varkappa_{ij}$ from the expression $J^{-1}(\Delta n_i A_{ij} - \Delta n_j A_{ji})$.

This method of calculation can be shown to be formally equivalent to the method described in Appendix 2. A numerical computation we have made leads to the same results.

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