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DIFFUSION COEFFIENTS AND INHOMOGENEOUS BIG BANG NUCLEOSYNTHESIS *

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Abstract

We study the effects of recently calculated baryon diffusion coefficients on the yields of primordial light elements in baryon-inhomogeneous big-bang models. The new coefficients are an improvement over previously used values in that they go to the correct nonrelativistic limit for neutron-electron scattering and give a more correct numerical value for the nucleon-nucleon scattering contribution. The largest effect of these new coefficients on nucleosynthesis is through neutron-proton scattering. We find that the somewhat larger value for D_{np} in the present work shifts the optimum separation distance between fluctuations, at which the effects of inhomogeneities are maximized, to slightly larger distance scales.

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There has been considerable recent interest [1–11] in the diffusion of baryons before, during, and after the epoch of primordial nucleosynthesis in the big bang. Baryon inhomogeneities might have been produced in the early universe (perhaps during the QCD transition [1,12], the electroweak transition [11], or by some other means, *cf.* ref. [12] and refs. therein). If such inhomogeneities were present, then the different diffusion lengths for neutrons and protons (once they obtain distinct identities at $t \sim 1$ s) could lead to the formation of high-baryon-density proton-rich regions and low-baryon-density neutron-rich regions from which the light-element nucleosynthesis yields can differ significantly from those of the standard homogeneous big bang.

In view of the importance of using light-element yields from the big bang to constrain the baryon-to-photon ratio as well as various cosmological and particle-physics theories [12,13], such inhomogeneous models must be examined seriously. It is therefore important to quantify the effects of baryon diffusion as accurately as possible. In this regard, it is of interest that recently there has been a calculation of the baryon diffusion coefficients by Banerjee and Chitre [14] in the lowest order Chapman–Enskog approximation to the relativistic kinetic theory. In this paper we study the effect of these new coefficients on the yields of primordial ^{2}H, ^{3}He, ^{4}He, and ^{7}Li in baryon inhomogeneous big-bang models [2–10], using the inhomogeneous nucleosynthesis code of ref. [6].

Since the diffusion of neutrons is much more important than protons until late in the big bang [2,6], we can ignore proton diffusion here. The effect of late-time expansion of the protons has been discussed previously [15] and is not likely to be significantly affected by the new diffusion coefficients.

The neutron-electron diffusion coefficient, as given by [14] is,

$$D_{ne} = \frac{3}{8}\sqrt{\frac{\pi}{2}}\frac{1}{n_e\sigma_t}\frac{K_2(z)}{z^{1/2}K_{5/2}(z)}\,(1-x_n), \tag{1}$$

where n_e is the total density of electrons and positrons, K_2 and $K_{5/2}$ are modified Bessel functions of order 2 and 5/2, and $z = m_e/T$. Here x_n is the neutron fraction of total particles [14], and can be neglected in the big bang. The transport cross section σ_t for the scattering of neutrons by electrons due to the interaction of their magnetic moments is $\sigma_t = 8 \times 10^{-31}\mathrm{cm}^2$ [2]. Previous work [2–10] has made use of the formula given by

Applegate, Hogan, and Scherrer (AHS) [2],

$$D_{ne}^{\mathrm{AHS}} = \frac{3\pi^2}{16m_e^3}\frac{1}{\sigma_t}\frac{ze^z}{1+3/z+3/z^2}, \tag{2}$$

which assumes a zero electron chemical potential, $\mu = 0$. Equation (1) is written explicitly in terms of n_e, and can be used for $\mu \neq 0$ as well. Both (1) and (2) are derived using relativistic Maxwell–Boltzmann (MB) statistics. The MB density for electrons+positrons is

$$n_e = \frac{2m_e^3}{\pi^2\hbar^3}\frac{1}{z^3}\cosh\frac{\mu}{T}\int_0^\infty k^2\exp(-\sqrt{k^2+z^2})dk. \tag{3}$$

Since

$$K_2(z) = \frac{1}{z^2}\int_0^\infty k^2\exp(-\sqrt{k^2+z^2}dk) \tag{4}$$

and

$$K_{5/2}(z) = \sqrt{\frac{\pi}{2}}\frac{1+3/z+3/z^2}{z^{1/2}e^z} \tag{5}$$

equations (1) and (2) turn out to be identical except for the factor $\cosh(\mu/T)$ in n_e.

At very high temperatures, $T \gtrsim m_e$, the $\mu = 0$ MB density is somewhat larger than the $\mu = 0$ Fermi–Dirac (FD) density,

$$n_e = \frac{2m_e^3}{\pi^2\hbar^3}\frac{1}{z^3}\int_0^\infty \frac{k^2 dk}{\exp(\sqrt{k^2+z^2})+1}. \tag{6}$$

For $\mu = 0$ and $T > 10^{10}$K, eq. (3) is larger than eq. (6) by a factor of 1.1. At these temperatures the n_e in our nucleosynthesis code is the FD result, and consequently we are using eq. (1) with eq. (6). In principle this is inconsistent, since eq. (1) is a strictly classical result. In practice, this difference is unimportant for our problem, and this approach is adequate. For $\mu = 0$ and $T < 10^9$K the relative difference between the two statistics is less than 10^{-3}.

For $\mu \neq 0$, however, n_e is always larger than in the $\mu = 0$ case, although at high temperatures the difference is insignificant. Once the temperature is low enough that the net electrons dominate over the thermal electron-positron pairs, eq. (1) must be used. In the early universe, this happens at a low enough temperature, so that nonrelativistic MB statistics can be used to obtain the electron density,

$$n_{e^\mp} = \frac{2}{\hbar^3}\left(\frac{m_e T}{2\pi}\right)^{3/2} e^{-m_e/T} e^{\pm\mu/T} \tag{7}$$

$$n_e \equiv n_{e^+} + n_{e^-} = \frac{4}{\hbar^3}\left(\frac{m_e T}{2\pi}\right)^{3/2} e^{-m_e/T} \cosh\frac{\mu}{T} \tag{8}$$

$$q_e \equiv n_{e^-} - n_{e^+} = \frac{4}{\hbar^3}\left(\frac{m_e T}{2\pi}\right)^{3/2} e^{-m_e/T} \sinh\frac{\mu}{T}. \tag{9}$$

Overall charge neutrality requires that the net electron density q_e be equal to the total density of free plus bound protons. Thus, one can avoid the necessity of determining the electron chemical potential μ in a nucleosynthesis calculation by rearranging equations (8) and (9),

$$n_e = \sqrt{\frac{16}{\hbar^6}\left(\frac{mT}{2\pi}\right)^3 e^{-2m_e/T} + q_e^2}. \tag{10}$$

In an $\Omega_b h_{50}^2 = 1$ universe this electron density begins to deviate significantly from the $\mu \approx 0$ approximation at $T_9 < 0.25$, past most of the nucleosynthesis activity. In inhomogeneous nucleosynthesis models the high-density regions also have higher net electron densities, so the expressions deviate at a somewhat higher temperature.

We calculated D_{ne} from eq. (1) in the early universe as a function of temperature for different comoving net electron densities. This is plotted in Fig. 1. The n_e used is the larger of eqs. (6) and (10). (At high temperatures the nonrelativistic formula (10) gives the smaller value, so this scheme picks the right approximation for each temperature).

The neutron-proton diffusion coefficient given by [14],

$$D_{np} = \frac{3\sqrt{\pi}}{4}\sqrt{\frac{T}{m_p}}\frac{1}{n_p\sigma_{np}}(1 - x_n), \tag{11}$$

is similar to that used by AHS,

$$D_{np}^{\mathrm{AHS}} = \frac{1}{\sqrt{3}}\sqrt{\frac{T}{m_n}}\frac{1}{n_p\sigma_{np}}, \tag{12}$$

to derive their final formula,

$$D_{np}^{\mathrm{AHS}} = \frac{6.53 \times 10^{10}}{1 - X_n}\frac{T_e^{1/2}}{\eta_8\sigma_{np}T_\nu^3}\frac{\mathrm{cm}^2}{\mathrm{s}}, \tag{13}$$

where $X_n = 1/6$, the neutron abundance just prior to the nucleosynthesis.

Equations (11) and (12) are essentially identical except that the numerical factor for the diffusion coefficient of ref. [14] is larger by $3\sqrt{3\pi}/4 \approx 2.3$. This factor can be traced to the difference between using an elementary mean-free-path method to estimate the diffusion coefficient *vs.* a velocity-distribution method as embodied in the Chapman–Enskog formalism [16]. However, ambiguities arise in eq. (11) from the mixing of classical and quantum mechanical expressions. Equation (11) comes from the Chapman–Enskog diffusion coefficient for hard-sphere classical scattering, for which the diffusion coefficient for a two-component gas of equal mass particles, 1&2, is [17],

$$D_{12} = \frac{3\sqrt{\pi}}{8}\sqrt{\frac{T}{m}}\frac{1}{n_1\sigma_{12}^{cl}}(1-x_2), \tag{14}$$

where σ_{12}^{cl}, is the classical hard-sphere cross section. Since the low-energy quantum mechanical cross section is twice the classical hard-sphere limit, σ_{12}^{cl} in eq. (14) was set to $\sigma_{np}/2$ in ref. [14] so that the classical formalism was adhered to as much as possible. On the other hand, there is no rigorous justification for this normalization without a purely quantum mechanical treatment of the velocity-distribution method which is beyond the scope of the present work. We point out that if σ_{np} is inserted into eq. (14) without renormalization then the resultant neutron-proton diffusion coefficient is only a factor of 1.15 different than the value derived from the mean-free path approximation and there would be no significant change between the present results and past nucleon diffusion calculations. However, since our purpose is to find the maximum effect which the new diffusion coefficients could have on previous conclusions, we adopt the normalization of ref. [14]. As we shall see below, even then, there is not much difference between the present nucleosynthesis yields and those of past calculations.

For the purpose of our numerical calculation, the cross-section for s-wave neutron-proton scattering is taken to be [2]

$$\sigma_{np} = \frac{\pi a_s^2}{(a_s k)^2 + (1-\frac{1}{2}r_s a_s k^2)^2} + \frac{3\pi a_t^2}{(a_t k)^2 + (1-\frac{1}{2}r_t a_t k^2)^2}, \tag{15}$$

where $a_s = -23.71$fm, $r_s = 2.73$fm, $a_t = 5.342$fm, and $r_t = 1.749$fm. For k, we use the thermal neutron momentum $\hbar k = \sqrt{3m_nT}$.

We plot D_{np}, from eq. (11), for different comoving proton densities in Fig. 1. The middle curve, $n_p/n_\gamma = 7 \times 10^{-9}$, would correspond to the critical baryon density $\Omega_b = 1$ for $H_0 = 50\mathrm{kms}^{-1}\mathrm{Mpc}^{-1}$, if the baryons were all protons. In the actual nucleosynthesis calculation the comoving proton density changes with time because of nuclear reactions and diffusion.

The effective neutron diffusion coefficient D_n is given by

$$\frac{1}{D_n} = \frac{1}{D_{ne}} + \frac{1}{D_{np}}, \tag{16}$$

where

$$\frac{1}{D_{ne}} = \frac{1}{D_{ne^-}} + \frac{1}{D_{ne^+}}. \tag{17}$$

From Fig. 1 we see that neutron-proton scattering dominates during the late part of the nucleosynthesis epoch, and for high baryon densities dominates during the entire nucleosynthesis epoch. It is clear from Fig. 1 that using equation (1) for D_{ne}, instead of equation (2), does not significantly affect the inhomogeneous nucleosynthesis yields, since the differences between eqs. (11) and (12) are manifested when the neutron diffusion coefficient is completely dominated by D_{np}.

Using both the old diffusion coefficients, equations (2) and (12), and the new, equations (1) and (11), we have calculated inhomogeneous nucleosynthesis yields for a model with an initially square-wave spherical inhomogeneity. We have chosen parameters which are close to those [8] which maximize the effects of baryon diffusion, i.e. an initial ratio of baryon densities, R, of $R = 10^3$, and a fraction, f_V, of the total volume initially occupied by the high density regions of $f_V = 1/64$. For the present baryon densities we use $\Omega_b h_{50}^2 = 0.1$ and 1.0. We also use $\tau_n = 888.6$s for the neutron lifetime [18] (half-life 10.266 min). The resulting abundances as a function of the distance scale of the inhomogeneity are shown in Fig. 2.

For the $\Omega_b h_{50}^2 = 1.0$ case, the results can be described simply. The new diffusion coefficients have shifted the abundance curves to larger distance scales by a factor of $\approx 1.5 \approx \sqrt{2.3}$. This is the effect of multiplying D_{np} by 2.3. For this high density case, D_{np} dominates, and D_{ne} does not matter. For the $\Omega_b h_{50}^2 = 0.1$ case, the effect is slightly smaller, since both D_{np} and D_{ne} are important during nucleosynthesis, and the latter is essentially unchanged at the relevant temperatures.

In the course of this work, we also discovered that the code used in ref. [6] contained a coding error in calculating D_{np}, causing it to be about a factor of 4 too small during nucleosynthesis. This had the opposite effect to that described above, shifting the results towards shorter distance scales by a factor of about 2. This explains a discrepancy between distances determined in refs. [6] and [8]. However, the basic conclusions regarding the difficulties of large Ω_b within the parameter space studied in ref. [6] remain unchanged.

The diffusion coefficients calculated using the relativistic kinetic theory do not seem to change appreciably the isotope yields obtained from inhomogeneous nucleosynthesis. Thus, the basic conclusions previously obtained should remain valid, except that the most favorable distance scale (producing low ^{4}He) is now found to be slightly larger. There was already a difficulty [19] in getting a long enough distance scale from the quark-hadron transition, so this modification is in the direction to make it even more difficult. However, the qualitative situation remains the same as summarized in refs. [6] and [8].

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References

[1] E. Witten, Phys. Rev. D30 (1984) 3037; M. Crawford, D.N. Schramm, Nature 298 (1982) 538.

[2] J.H. Applegate, C.J. Hogan and R.J. Scherrer, Phys. Rev. D 35 (1987) 1151.

[3] C. Alcock, G.M. Fuller and G.J. Mathews, Astrophys. J. 320 (1987) 439;
G.M. Fuller, G.J. Mathews and C.R. Alcock, Phys. Rev. D 37 (1988) 1380.

[4] H. Kurki-Suonio, R.A. Matzner, J.M. Centrella, T. Rothman and J.R. Wilson, Phys. Rev. D 38 (1988) 1091.

[5] R.A. Malaney and W.F. Fowler, Astrophys. J. 333 (1988) 14.

[6] H. Kurki-Suonio and R.A. Matzner, Phys. Rev. D 39 (1989) 1046; D 42 (1990) 1047; H. Kurki-Suonio, R.A. Matzner, K.A. Olive and D.N. Schramm, Astrophys. J. 353 (1990) 406.

[7] N. Terasawa and K. Sato, Prog. Theor. Phys. 81 (1989) 254; 81 (1989) 1085; Phys. Rev. D 39 (1989) 2893.

[8] G.J. Mathews, B.S. Meyer, C.R. Alcock and G.M. Fuller, Astrophys. J. 358 (1990) 36.

[9] B.S. Meyer, C.R. Alcock, G.J. Mathews and G.M. Fuller, Phys. Rev. D 43 (1991) 1079.

[10] H. Reeves, Phys. Rep. 201 (1991) 335.

[11] L. McLerran, Phys. Rev. Lett. 62 (1989) 1075. (1990) 1.

[12] R.A. Malaney and G.J. Mathews, Phys. Rep. (1991) in press.

[13] T.P. Walker, G. Steigman, D.N. Schramm, K.A. Olive and H.-S. Kang, Astrophys. J. 376 (1991) 51, and references therein.

[14] B.Banerjee and S.M. Chitre, Phys. Lett. B 258 (1991) 250.

[15] C.R. Alcock, D.S. Dearborn, G.M. Fuller, G.J. Mathews, and B.S. Meyer, Phys. Rev. Lett. 64 (1990) 2607.

[16] S. Chapman and T.G. Cowling, *The Mathematical Theory of Non-Uniform Gases*, Cambridge University Press, Cambridge, 1970.

[17] S.R. de Groot, W.A. van Leeuwen and Ch.G. van Weert, *Relativistic Kinetic Theory*, North-Holland, Amsterdam, 1980.

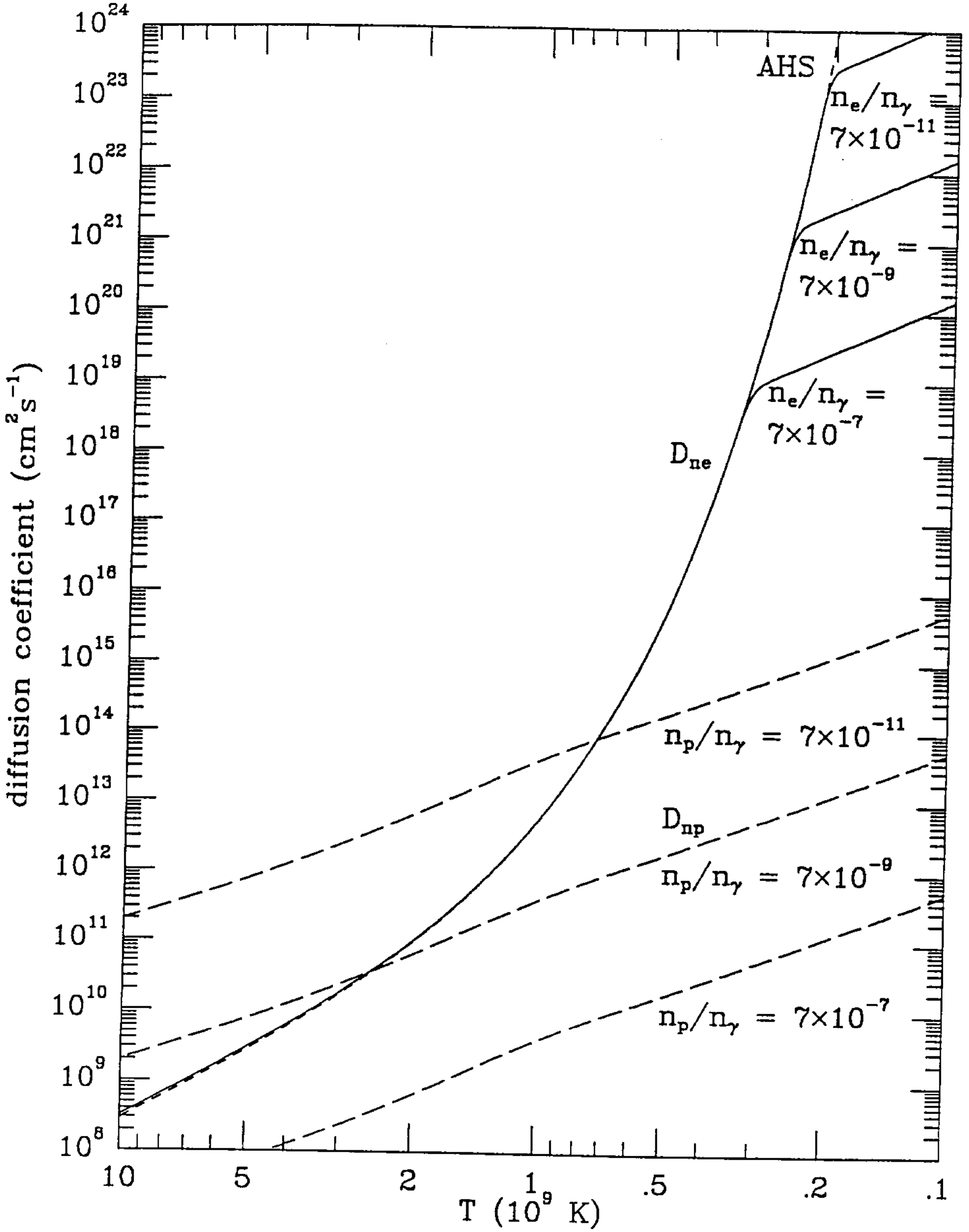
[18] Particle Data Group, J.J. Hernández et al., Phys. Lett. B 239 (1990) 1.

[19] K. Kajantie, L. Kärkkäinen, and K. Rummukainen, Nucl. Phys. B 333 (1990) 119.

Figure captions

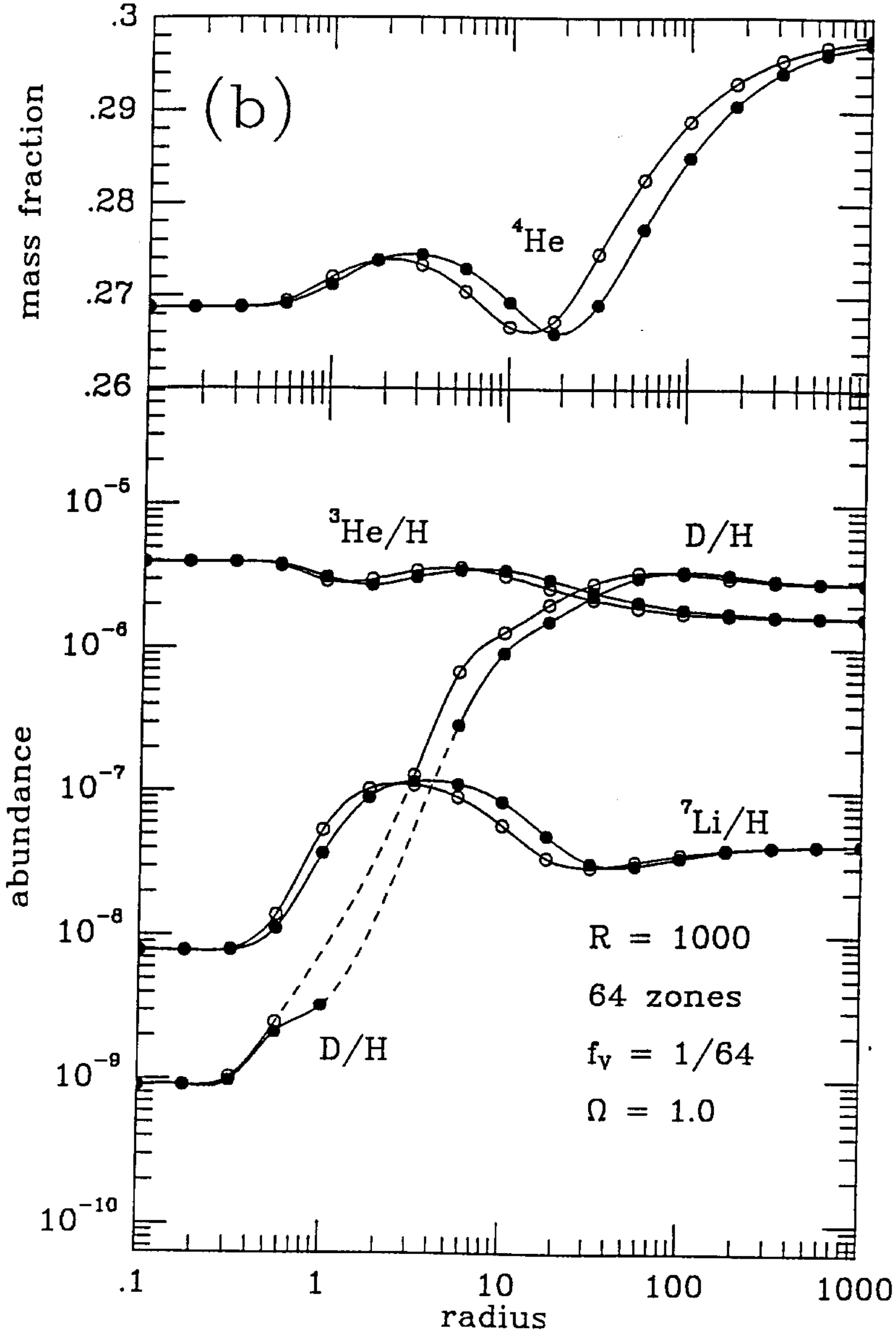
Fig. 1. The neutron-electron (D_{ne}, solid lines) and neutron-proton (D_{np}, long-dashed lines) diffusion coefficients as a function of temperature for different comoving net electron (n_e/n_γ) and proton (n_p/n_γ) number densities. The short-dashed line is the $\mu = 0$ approximation to D_{ne} due to AHS [2]. The smaller of D_{ne} and D_{np} dominates the effective neutron diffusion coefficient, D_n.

Fig. 2. Inhomogeneous nucleosynthesis yields as a function of distance scale. The distance is given in light-hours today, which corresponds to 1.5 m at $T = 100$ MeV, and is measured from the center of the high-density region to the center of the low-density region of a spherical cell. The initial high/low baryon density ratio is $R = 10^3$ and the high density volume fraction is $f_V = 1/64$. The open circles (o) are results obtained using the AHS diffusion coefficients, the filled circles (•) are obtained with the new diffusion coefficients. (a) For $\Omega_b h_{50}^2 = 0.1$. (b) For $\Omega_b h_{50}^2 = 1.0$. For (b) the numerical results are uncertain for deuterium where its dependence on the distance scale is the steepest (indicated with the dashed line). The main conclusion from this study is that the new diffusion coefficients shift the results to longer distance scales by a factor of ≈ 1.5.



diffusion coefficient (cm^{2}s^{-1})
T (10^9 K)
AHS
n_e/n_γ = 7×10^{-11}
n_e/n_γ = 7×10^{-9}
n_e/n_γ = 7×10^{-7}
D_{ne}
n_p/n_γ = 7×10^{-11}
D_{np}
n_p/n_γ = 7×10^{-9}
n_p/n_γ = 7×10^{-7}

Fig. 1



(b)
mass fraction
.3
.29
.28
.27
.26
^{4}He
^{3}He/H
D/H
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
abundance
^{7}Li/H
D/H
R = 1000
64 zones
f_v = 1/64
Ω = 1.0
.1
1
10
100
1000
radius

Fig. 2