Triple e^-pn collisions and primordial formation of deuterons

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The electron-catalysed nonradiative fusion of the proton and neutron, $e^- + p + n \to d + e^-$, is discussed within the framework of the primordial nucleosynthesis of light nuclei. Comparing the reaction rate of this three-particle process and that of its radiative counterpart reaction $p + n \to d + \gamma$, we show that the triple-collision plays a less significant role in the formation of deuterons at the plasma temperatures investigated.

Introduction

The theory of Big Bang nucleosynthesis is one of the most important parts of modern cosmology. By relating the abundances of light elements in the contemporary universe to the processes which took place during the first few minutes after the Big Bang, a theory of primordial nucleosynthesis enables astrophysicists to investigate various assumptions about physical conditions prevailing at that time.[1] In particular, primordial production of deuterium is very sensitive to the baryon density and therefore predictions and measurements of deuterium abundance can be used to infer the density of baryons in the early universe. Besides this, the importance of studying primordial processes of deuterium formation follows from the fact that they represent the so-called 'bottleneck' for synthesis of all other elements.

The standard model of Big Bang nucleosynthesis is able to account for many (although not all) conditions of the primordial plasma, the remaining discrepancies may be attributed either to wrong assumptions about these conditions, or to the inadequacy of the model itself. It is therefore important to scrutinize all the simplifications and approximations of the model before drawing conclusions. In this paper, we are concerned with one such simplifications, namely, the omission of triple collisions in the processes of deuteron formation.

In the standard model,[2] it is assumed that the formation of light nuclei mainly occurs through the *pp*-chain, which begins with the synthesis of deuterons in the processes

$$\mathrm{p}+\mathrm{p} \;\rightarrow\; \mathrm{d}+\mathrm{e}^+ + \nu_\mathrm{e}\,, \tag{1}$$

$$\mathrm{p}+\mathrm{e}^- +\mathrm{p} \;\rightarrow\; \mathrm{d}+\nu_\mathrm{e} \tag{2}$$

involving strong and weak forces, and in the strong-electromagnetic reaction

$$\mathrm{n}+\mathrm{p} \rightarrow \mathrm{d}+\gamma\,. \tag{3}$$

The next step is the radiative capture of protons by deuterons

$$\mathrm{p}+\mathrm{d} \rightarrow {}^3\mathrm{He}+\gamma\,.$$

Then, the nucleosynthesis is assumed to continue via various two-body reactions such as

$$^3\mathrm{He}+{}^3\mathrm{He} \;\rightarrow\; {}^4\mathrm{He}+\mathrm{p}+\mathrm{p}\ ,$$

$$^3\mathrm{He}+{}^4\mathrm{He} \;\rightarrow\; {}^7\mathrm{Be}+\gamma\,.$$

Except for the so-called pep reaction (2), three-body collisions are omitted in the standard model. This is done on the grounds that they are less frequent. It is known, however, that in three-body collisions there are more ways to satisfy the conservation laws (such as conservation of parity, angular momentum, and isospin) than in the two-body processes. As a result, three-body collisions are less restricted by various selection rules and therefore might make a noticeable contribution to the net production of certain nuclei, when both two- and three-body initial states lead to the same final product. This kinematical difference between two- and three-body initial states means that some binary nuclear reactions suppressed by conservation laws can be eased due to the presence of a third particle.

To shed some light on the role played by triple collisions in the primordial formation of light nuclei, explicit calculations of three-body nuclear reactions are needed. Several articles on this matter have been published in recent years.[3–6] In the present paper, we compare the rates of the three-body non-radiative process

$$\mathrm{e}^- +\mathrm{n}+\mathrm{p} \rightarrow \mathrm{d}+\mathrm{e}^- \tag{5}$$

and the corresponding two-body reaction (3), which is included in the standard model of Big Bang nucleosynthesis.

Reaction rate

According to the standard model,[1] the primordial formation of nuclei started in $\sim 10^{-2}$ seconds after the Big Bang, with an average energy per particle of ~10 MeV and the matter density $\sim 10^9$ g/cm^3. Big Bang nucleosynthesis lasted about 100 seconds until the temperature dropped to ~0.1 MeV and the density to ~10 g/cm^3. In the early stages, the primordial plasma was totally ionized, which means that the electrons were not associated with specific nuclei and can be considered as moving in continuum states, i.e. freely among the nuclei. Because of the high density, the average distances between the particles were small and the nuclei were closely surrounded by electrons. When two nucleons collided, there was always an electron nearby. The triple-collision processes (5), may therefore have made a noticeable contribution to the formation of deuterons. To assess this contribution, we need to calculate the average reaction rate for all possible reactions (5), starting from different initial states characterized by different momenta of colliding particles.

Let $\Psi_\mathbf{p}$ be the wave function of the relative motion of the *pn*–pair with momentum $\mathbf{p}$ and let $\mathbf{k}$ be the momentum of the electron with respect to this pair. Let η represent a set of the discrete quantum numbers characterizing the spin–isospin state of the three particles. Then, for the three-body collision process (5) with the initial and final energies E_i and E_f, the reaction rate per unit volume per second is defined by[7]

$$\mathcal{R}_3(\mathbf{p},\mathbf{k},\eta \;\longrightarrow\; \mathbf{k}',\eta') = \frac{1}{4\pi^2}\delta(E_f-E_i)\left|\langle\Psi_d,\mathbf{k}',\eta'|T|\Psi_\mathbf{p},\mathbf{k},\eta\rangle\right|^2 n_p n_n n_e\,, \tag{6}$$

where the states in the continuum are normalized as

$$\langle\Psi_{\mathbf{p}'},\mathbf{k}'|\Psi_\mathbf{p},\mathbf{k}\rangle = (2\pi)^6\delta(\mathbf{k}'-\mathbf{k})\delta(\mathbf{p}'-\mathbf{p})\,,$$

T is the transition operator, Ψ_d is the wave function of deuteron, and n_p, n_n, and n_e represent the corresponding particle densities. It is a standard assumption[1] that in primordial plasma at temperature θ, the momenta $\mathbf{p}$ and $\mathbf{k}$ were distributed according to Maxwell's law

$$N_\mathbf{p}(\theta) \;=\; (2\pi\mu\kappa\theta)^{-3/2}\exp\left(-\frac{p^2}{2\mu\kappa\theta}\right),$$

$$N_\mathbf{k}(\theta) \;=\; (2\pi m\kappa\theta)^{-3/2}\exp\left(-\frac{k^2}{2m\kappa\theta}\right),$$

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where $N_{\mathbf{p}}(\theta)$ and $N_{\mathbf{k}}(\theta)$ are the probability densities, μ is the proton–neutron reduced mass, m is the electron mass, and κ is the Boltzmann constant. We are concerned with the total rate of the transition from an initial state with any $(\mathbf{p}, \mathbf{k}, \eta)$ to a final state with all possible $\mathbf{k}', \eta'$. Thus the reaction rate (6) must be averaged over the initial quantum numbers $\mathbf{p}$, $\mathbf{k}$, η and integrated over the final quantum numbers $\mathbf{k}', \eta'$. The averaging over $\mathbf{p}$ and $\mathbf{k}$ is achieved by summing-up the $\mathcal{R}_3$ for all possible values of these momenta with the weight factors $N_{\mathbf{p}}(\theta)$ and $N_{\mathbf{k}}(\theta)$ corresponding to their probabilities, i.e.

$$\langle \mathcal{R}_3 \rangle_\theta = \frac{1}{M} \sum_{\eta\eta'} \int\int\int d\mathbf{p} d\mathbf{k} d\mathbf{k}' \, \mathcal{R}_3(\mathbf{p}, \mathbf{k}, \eta \longrightarrow \mathbf{k}', \eta') N_{\mathbf{p}}(\theta) N_{\mathbf{k}}(\theta), \qquad (7)$$

where M is the number of possible (initial) spin–isospin states.

Similarly to two-body reaction theory where the average reaction rate $\langle \mathcal{R}_2 \rangle_\theta$ is written as a product of $\langle \sigma v \rangle_\theta$ (which is called the reaction rate per particle pair) and the particle densities,[2]

$$\langle \mathcal{R}_2 \rangle_\theta = n_1 n_2 \langle \sigma v \rangle_\theta \, ,$$

the three-body reaction rate $\langle \mathcal{R}_3 \rangle_\theta$ can also be factorized in the same manner,

$$\langle \mathcal{R}_3 \rangle_\theta = n_p n_n n_e \langle \Sigma \rangle_\theta . \qquad (8)$$

Indeed, according to (6) and (7)

$$\langle \Sigma \rangle_\theta = \frac{1}{4\pi^2 M} \sum_{\eta\eta'} \int\int\int d\mathbf{p} d\mathbf{k} d\mathbf{k}' \, \delta(E_f - E_i) \times \left| \langle \Psi_d, \mathbf{k}', \eta' | T | \Psi_{\mathbf{p}}, \mathbf{k}, \eta \rangle \right|^2 N_{\mathbf{p}}(\theta) N_{\mathbf{k}}(\theta). \qquad (9)$$

Transition amplitude

The motion of the nucleons is slow compared to that of the electron and thus can be treated adiabatically. Moreover, for the electron to participate in the three-body reaction (5), the two heavy particles (nucleons) must be close to each other when the electron arrives. Therefore, the transition from the initial to the final state can be viewed as the following two-step process

$$|\mathbf{p}, \mathbf{k}\rangle \stackrel{V_{pn}}{\Longrightarrow} |\Psi_{\mathbf{p}}, \mathbf{k}\rangle \stackrel{V_{pe}}{\Longrightarrow} |\Psi_d, \mathbf{k}'\rangle,$$

where V_{pn} and V_{pe} are the proton-neutron and proton-electron potentials. Therefore, instead of the transition

$$|\mathbf{p}, \mathbf{k}\rangle \stackrel{V_{pn}+V_{pe}}{\Longrightarrow} |\Psi_d, \mathbf{k}'\rangle$$

caused by both V_{pn} and V_{pe}, in the adiabatic approximation, we may consider the transition

$$|\Psi_{\mathbf{p}}, \mathbf{k}\rangle \stackrel{V_{pe}}{\Longrightarrow} |\Psi_d, \mathbf{k}'\rangle \, ,$$

where the interaction V_{pn} is already taken into account by using the scattering state $\Psi_{\mathbf{p}}$ instead of the plane wave $|\mathbf{p}\rangle$.

The adiabatic approximation also means that the transition operator T in Equation (6) can be replaced by the fixed scatterer T-matrix defined as

$$\tilde{T}(z) = V_{pe} + V_{pe} \frac{1}{z - h_0} \tilde{T}(z), \qquad (10)$$

where z is the total energy and h_0 is the kinetic energy operator associated with the momentum $\mathbf{k}$ of the electron.

As is customary in this kind of calculation,[3] the Coulomb interaction between the proton and the electron can be treated perturbatively, which leads to the following series expansion for the transition operator

$$\tilde{T}(z) = V_{pe} + V_{pe} \frac{1}{z - h_0} V_{pe} + V_{pe} \frac{1}{z - h_0} V_{pe} \frac{1}{z - h_0} V_{pe} + \cdots . \qquad (11)$$

For typical densities of the primordial plasma, the average potential energy $\langle V_{pe} \rangle$ is 10 eV, whereas the kinetic energy of the electrons is three orders of magnitude higher. This means that the series (11) should converge very fast and we can thus retain only the Born term. In other words,

$$T \approx V_{pe} .$$

Therefore, instead of (9), we have

$$\langle \Sigma \rangle_\theta \approx \frac{1}{4\pi^2 M} \sum_{\eta\eta'} \int\int\int d\mathbf{p} d\mathbf{k} d\mathbf{k}' \, \delta(E_f - E_i) \times \left| \langle \Psi_d, \mathbf{k}', \eta' | V_{pe} | \Psi_{\mathbf{p}}, \mathbf{k}, \eta \rangle \right|^2 N_{\mathbf{p}}(\theta) N_{\mathbf{k}}(\theta) , \qquad (12)$$

which is the final formula used in our calculations. To calculate $\Psi_{\mathbf{p}}$ and Ψ_d entering this integral, we numerically solved the corresponding Schrödinger equation with the *S*-wave Malfliet-Tjon *NN* potential[8] using the Jost function method.[9] Then the multidimensional integral (12) was evaluated using the Simpson's $\frac{3}{8}$ Rule.[10]

Results and conclusions

For the sake of comparison, we considered the reaction rates

$$\langle \mathcal{R}_2 \rangle_\theta = n_p n_n \langle \sigma v \rangle_\theta$$

and

$$\langle \mathcal{R}_3 \rangle_\theta = n_p n_n n_e \langle \Sigma \rangle_\theta$$

for both the two-body and three-body processes (3) and (5) in the same region of the plasma temperature. Radiative capture described by (3) has been studied for many decades and its theory can be found in textbooks on nuclear physics. To calculate $\langle \sigma v \rangle_\theta$, we used the formulae given in one of them.[11]

Once $\langle \sigma v \rangle_\theta$ and $\langle \Sigma \rangle_\theta$ are calculated, the relative contribution of the triple non-radiative capture to the formation of deuterons can be estimated by calculating the ratio

$$\frac{\langle \mathcal{R}_3 \rangle_\theta}{\langle \mathcal{R}_2 \rangle_\theta} = \frac{\langle \Sigma \rangle_\theta}{\langle \sigma v \rangle_\theta} \, n_e \, , \qquad (13)$$

in which the (poorly known) densities n_p and n_n are cancelled out.

Equation (13) shows that the contribution of the reaction (5) is proportional to the density of electrons. This density consists of two parts, the first being the density of 'background' electrons (one per proton) and the second the density of electrons emerging from numerous electron positron pairs continuously produced by strong electromagnetic radiation. The second part, corresponding to the 'pair' electrons, is known to be dominant under the primordial nucleosynthesis conditions.[12] For this reason, we used the temperature-dependent n_e[13]

$$n_e = \frac{1}{\pi^2} \left(\frac{mc}{\hbar} \right)^3 \left(\frac{\theta}{mc^2} \right) K_2(mc^2/\theta), \qquad (14)$$

which describes the density of the 'pair' electrons. The modified Bessel function K_2 in this equation makes this density extremely high at the very beginning of the nucleosynthesis, but it exponentially vanishes when the plasma cools down. This means that the three-body processes (5) might give a noticeable contribution to the production of deuterons at least at high values of θ.

The results of our calculations for various plasma temperatures are given in Table 1. It is seen that, unlike in the case of other three-body fusion reactions,[3,5,6] the triple collisions (5) play a minor role compared to that of binary reactions (3). This finding can be attributed mainly to the fact that the *np* system, unlike the other systems considered, has no Coulomb repulsion. Indeed, all the three-body reactions considered earlier (such as $e^- + {}^3He + {}^4He \rightarrow e^- + {}^7Be$ in ref. 6) involve positively charged nuclei. The presence of the electron in close vicinity to the nuclei reduces the repulsion between them and thus facilitates fusion. This, of course, has no effect on the *np* system.

Table 1. Temperature dependence of ratio of the triple to binary reaction rates for the processes leading to formation of deuterons in primordial plasma.

θ (keV)	θ (10^9 K)	n_e (cm^{-3})	$\mathcal{R}_3/\mathcal{R}_2$
10	0.116	0.38×10^{6}	0.478×10^{-11}
20	0.232	0.13×10^{18}	0.171×10^{-9}
30	0.348	0.12×10^{22}	0.715×10^{-9}
40	0.464	0.13×10^{24}	0.166×10^{-8}
50	0.580	0.24×10^{25}	0.302×10^{-8}
60	0.696	0.17×10^{26}	0.482×10^{-8}
70	0.812	0.74×10^{26}	0.712×10^{-8}
80	0.928	0.23×10^{27}	0.999×10^{-8}
90	1.044	0.55×10^{27}	0.135×10^{-7}
100	1.160	0.11×10^{28}	0.177×10^{-7}
110	1.277	0.21×10^{28}	0.226×10^{-7}
120	1.393	0.35×10^{28}	0.282×10^{-7}
130	1.509	0.55×10^{28}	0.348×10^{-7}
140	1.625	0.81×10^{28}	0.421×10^{-7}
150	1.741	0.11×10^{29}	$0.504 \times 10^{-}$
160	1.857	0.16×10^{29}	0.596×10^{-7}
170	1.973	0.21×10^{29}	0.697×10^{-7}
180	2.089	0.26×10^{29}	0.808×10^{-7}
190	2.205	0.33×10^{29}	0.928×10^{-7}
200	2.321	0.41×10^{29}	0.106×10^{-6}
210	2.437	0.50×10^{29}	0.120×10^{-6}
220	2.553	0.60×10^{29}	0.135×10^{-6}
230	2.669	0.71×10^{29}	0.151×10^{-6}
240	2.785	0.83×10^{29}	0.167×10^{-6}
250	2.901	0.96×10^{29}	0.185×10^{-6}
260	3.017	0.11×10^{30}	0.204×10^{-6}
270	3.133	0.13×10^{30}	0.223×10^{-6}
280	3.249	0.14×10^{30}	0.244×10^{-6}
290	3.365	0.16×10^{30}	0.265×10^{-6}
300	3.481	0.18×10^{30}	0.287×10^{-6}

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