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TEMPERATURE EFFECTS ON NUCLEAR MASSES, REACTIONS AND ABUNDANCES

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Abstract

Nuclear reactions occurring in astrophysical environments are influenced by the masses and energies of the nuclei involved, as well as the temperature of the surrounding environment. It is noteworthy to observe the relationship between the excitation energies of nuclei and the temperature of the environment in which the nuclei are present. Therefore, it is reasonable to consider the temperature dependence of masses in astrophysical environments. However, it is common in the literature to treat nuclear masses as constant regardless of temperature. In this study, we will explore the effects of temperature on nuclear masses and investigate how this variation impacts the relevant nuclear reaction rates in the context of big bang nucleosynthesis. By considering the temperature dependence of masses, we aim to gain a deeper understanding of the changes in reaction rates that occur in astrophysical scenarios.

Resumen

Las reacciones nucleares en ambientes astrofísicos dependen de las masas, las energías y la temperatura del entorno. Al observar la relación entre las energías de excitación de los núcleos y la temperatura del ambiente en el que se encuentran, es razonable considerar la dependencia de la temperatura en las masas nucleares en entornos astrofísicos. En este trabajo, se incluyen los efectos de la temperatura en las masas nucleares y se examina cómo las tasas de reacción nuclear relevantes cambian en el contexto de la nucleosíntesis del Big Bang.

Keywords: Nuclear reactions, reverse reaction rates, primordial nucleosynthesis
Palabras clave: Reacciones nucleares, tasa de reacción reversa, nucleosíntesis primordial

I. INTRODUCTION

Big Bang nucleosynthesis (BBN) or primordial nucleosynthesis is responsible for the production of light elements. The process took place few seconds after the Big Bang and lasted for around 20 minutes when the temperature of the universe was not high enough to allow more nuclear reactions. BBN is an early test of the standard cosmological model. Comparisons of observed and predicted abundances of the light elements show great agreement for most of them, with the exception of ^{7}Li. The predicted abundance of ^{7}Li is three times higher than the observed abundance (Bertulani & Shubhchintak, 2018; Hou et al., 2019).

Nuclear reactions in this astrophysical environment involve temperatures high enough to excite nuclei above their ground states. The energy of an excited nucleus can be related to a temperature-dependent binding energy and, hence, also a temperature-dependent mass (Davidson, 1993). Calculations of thermonuclear reaction rates typically take into account the temperature dependence through a Maxwell-Boltzmann factor, while also incorporating the existence of excited states of nuclei. However, the explicit temperature dependence of masses is not considered.

For example, Caughlan (1998) provides a list of analytical expressions for nuclear reaction rates, where these expressions depend on temperature. However, the expressions for the reverse reaction rates are simplified using the reciprocity theorem. This theorem allows the forward and reverse reaction rates to be related through an exponential function with the Q-value of the reaction. Conventionally, the Q-values are defined based on the ground state masses, which implies an incomplete inclusion of excited nuclei in the reaction. In this work, we demonstrate how the reverse reaction rate of a reaction that produces ^{7}Li can change when we consider this effect.

Furthermore, without delving into a complicated network calculation, we assume nuclear statistical equilibrium (NSE) and include temperature-dependent binding energies to calculate the

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abundance of lithium at different temperatures. This example provides an idea of the changes in abundance that can be obtained by incorporating temperature-dependent binding energies. The present work serves as a starting point to determine if further investigation in this direction, with more accurate inputs and a sophisticated network calculation, is worth pursuing.

II. FORMALISM

To consider the temperature effects in the nuclear masses we begin by expressing the mass of an excited nucleus as $m_A^* = m_A + E^*$ so that with $m_A = Z\ m_p + N\ m_n - |E_b|$, and $m_A^* = Z\ m_p + N\ m_n + E^* - |E_b|$, we can define the binding energy of the excited nucleus as $|E_b^*| = |E_b| - E^*$ which is obviously less than the binding energy of the nucleus in its ground state. Now we need a relation between the plasma temperature and the excitation energy. At a given temperature, we find the average excitation energy as follows (Davidson, 1993):

$$E^*(T) = \frac{\sum_i^{E_m} E_i^* g_i \exp(-E_i^*/k_b T) + \int_{E_m}^{\infty} E\rho(E)\exp(-E/k_b T)\,dE}{\sum_i^{E_m} g_i \exp\left(-E_i^*/k_b T\right) + \int_{E_m}^{\infty} \rho(E)\exp(-E/k_b T)\,dE} \tag{1}$$

where $\rho(E)$ is the density of states and E_m is the highest known excited state of the nucleus. Having related the average excitation energy with temperature in this manner, we now rewrite, $|E_b^*| = |E_b| - E^*$ mentioned above as

$$|E_b(T)| = |E_b(0)| - E^*(T) \tag{2}$$

thus obtaining a temperature dependent mass given by, $m_A(T) = Z\ m_p + N\ m_n - |E_b(T)|$. Since our calculations involve only light nuclei, we will use the density of states proposed in Le Couteur, 1959:

$$\rho(E) = \exp\left(2[a(E)]^{1/2}\right) \tag{3}$$

We take the level density parameter, a, from Murata (2001):. However, there are some nuclei that are not given in the document, for them we make a prediction using Ordinary Least Square (OLS) fit with the information available for light nuclei. The model has the following expression:

$$a = -1.508658 + 0.264372A.$$

As noted above, having an expression for average excitation energy, we can define the nuclear mass as:

$$m(A, Z, T) = m(A, Z, 0) + E^*(T). \tag{4}$$

With the masses depending on temperature, we calculate the new Q-values and use the expression for reactions rates from Caughlan (1998). By the reciprocity theorem, for a reaction 1 + 2 → 3 + 4, the reverse reaction rate, $\langle\sigma_{34}\rangle$, is related to the forward reaction rate, $\langle\sigma_{12}\rangle$, as follows:

$$\langle\sigma_{34}\rangle = \langle\sigma_{12}\rangle f(T)\exp(-Q/k_b T),$$

where $f(T)$ is a function of temperature that changes with the reactions, k_b is the Boltzmann constant and Q is the Q-value of the nuclear reaction. According to Eq. (2) and Eq. (4), the mass of a nucleus depends on the temperature, and since the Q-value is defined as the difference of masses, it should depend on the temperature as well. The ratio χ gives the relation between the reverse reactions including and not including this additional effect of temperature.

$$\chi = \frac{exp(-Q(T)/k_b T)}{exp(-Q(0)/k_b T)} \tag{5}$$

Using the thermodynamic equilibrium tools, we can evaluate relative abundances without going through the network calculations. Kinetic equilibrium implies (Kolb & Turner, 1994):

$$n_A = g_A \left(\frac{m_A T}{2\pi}\right)^{3/2} \exp\left(\frac{\mu_A - m_A}{T}\right). \tag{6}$$

If the plasma is in chemical equilibrium, we can relate the chemical potential of the nucleons as:

$$\mu_A = Z\mu_p + (A-Z)\mu_n. \tag{7}$$

With Eq. (6) and Eq. (7), we can write the abundance of species A as:

$$n_A = g_A A^{3/2} 2^{-A} \left(\frac{2\pi}{m_N k_b T}\right)^{3(A-1)/2} n_p^Z n_n^{A-Z} \exp(E_b/T), \tag{8}$$

where E_b is the nuclear binding energy.

Besides the direct dependence on temperature in the exponential factor, the binding energy also has a temperature dependence since it is related with the nuclear mass. If we assume that the terms multiplying the exponential do not depend on temperature, then we can study the factor of this new abundance relative to the non-temperature-dependent one through:

$$\frac{n_A^T}{n_A} = \exp\left(\frac{E_b(T) - E_b(0)}{k_b T}\right) \tag{9}$$

III. RESULTS AND DISCUSSION

In this section we show how the reverse reaction and the equilibrium abundance changes when we include the temperature effect that comes from the inclusion of excited nuclei. For the reaction $^3He(t,\gamma)^7Li$, the forward reaction rate is given by Caughlan (1998):

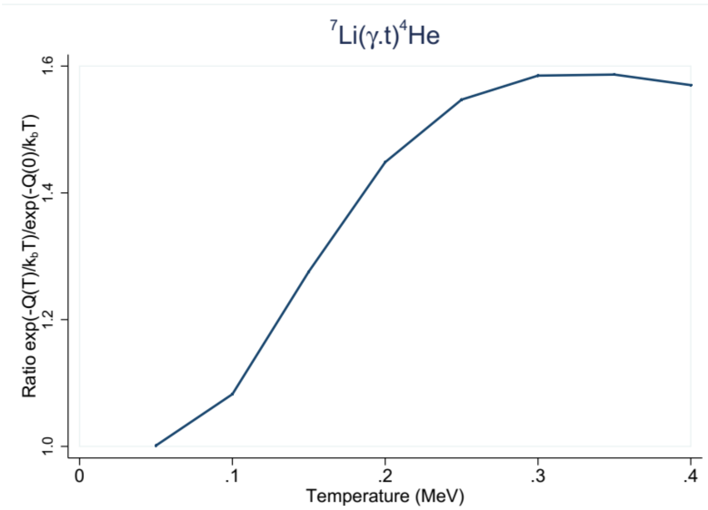
$$\langle\sigma_{12}\rangle = \frac{8.67 \times 10^5}{T_9^{2/3}} \exp\left(-8.080/T_9^{1/3}\right) \times \left(1 + 0.052T_9^{1/3} - 0.448T_9^{2/3} - 0.165T_9 + 0.144T_9^{4/3} + 0.134T_9^{5/3}\right)$$

and the reverse reaction rate is:

$$\langle\sigma_{34}\rangle = \langle\sigma_{12}\rangle 1.11 \times 10^{10} T_9^{3/2} \exp(-Q/k_b T)$$

Here $T^9 = T \times 10^9$ K. The reverse reaction will destroy lithium to produce more ^{4}He and ^{3}H. In Figure 1 we show the factor χ (Eq. (5)) for the reverse reaction with and without inclusion of the temperature effects:

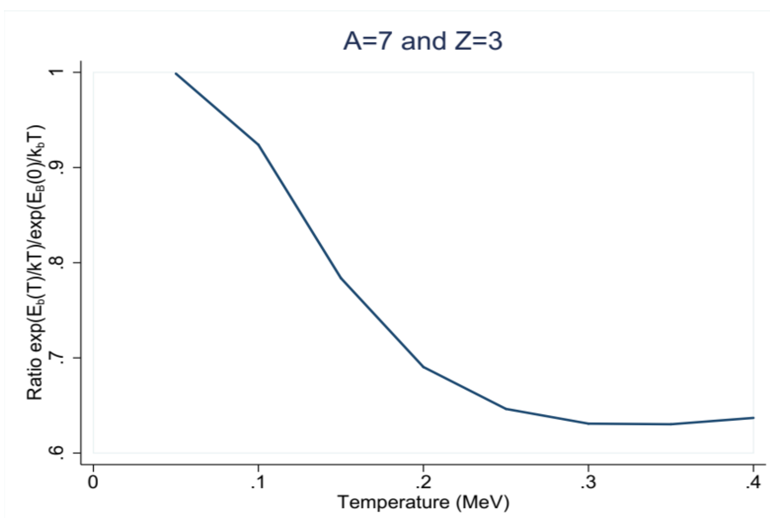
Figure 1.
Ratio of reverse reaction



We can observe that for temperatures between 0 and 0.3 MeV, ^{7}Li is being destroyed faster than it would by using the ground states Q-values. This means that lithium will probably be less abundant but at the same time there is more helium and tritium to perform more reactions.

Figure 2 shows the relation described in Eq. (9) for the case of nuclear statistical equilibrium.

Figure 2.
Ratio of equilibrium abundances



Here, we observe that the new equilibrium abundance is consistently lower than the abundance calculated without including the temperature effects. This reduction can lead to an approximate 10% change in abundance around a temperature of 70 keV, where the production of ^{7}Li becomes significant.

In this work, we demonstrated the consideration of temperature effects in nuclear reaction rates. We provided an example of an analytical forward and reverse reaction rate and examined the impact of including temperature effects using the reverse reaction definition and the nuclear statistical equilibrium abundance. In both cases, we observed a small but significant change compared to the original results.

However, a realistic calculation of abundance would require the consideration of all possible reactions and their reverse reactions within a network calculation involving coupled differential equations. Therefore, while Fig. 1 does not directly provide information about abundance, it indicates the presence of some change that may or may not cancel out in the network calculations.

The predictions of ^{7}Li abundance in the literature are three times higher than the observed values. This work demonstrates how a simple calculation can modify the destruction of lithium and the equilibrium abundance, providing an insight into the direction of these changes. However, to determine the net impact on abundances, it is necessary to develop a Big Bang Nucleosynthesis network that incorporates this temperature effect.

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