Temperature dependent corrections in nucleosynthesis

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1 Introduction

Nuclear reactions in astrophysical environments depend on the masses, energies of the nuclei involved as well as the temperature of the surroundings. Noting the relation between excitation energies of nuclei and the temperature of the environment where the nuclei are found, it seems reasonable to consider the temperature dependence of masses in astrophysical environments. In the literature, usually, nuclear masses are considered to be constant at all temperatures. However given the energy-mass relation, it is appropriate to consider the effect of the temperature on the masses (Davidson et al. 1994) through the excitation energies at elevated temperatures. The temperature dependent masses in turn lead to temperature dependent Q values and binding energies (Ohnishi 1973) which decrease with increasing temperature.

In a fully ionized stellar plasma, electrons are attracted to a particular nucleus polarizing its neighborhood, reducing the repulsive Coulomb barrier between nuclei and affecting the reaction rates and tunneling probabilities. This effect is called electron screening and it leads to a correction in the nuclear reaction rate calculations. The temperature dependence of screening effects are usually incorporated in an approximate way in the calculation of nuclear reaction rates. We plan to investigate the available approximate equations arising from the Feynman Metropolis Teller equation and solve one of them, for example, the Thomas-Fermi equation in order to incorporate the temperature dependent screening effects in the best possible way.

In this work we will evaluate some effects of temperature on the reactions rates through masses and through electron screening. It is expected that changing the reaction rates will alter the distribution of abundances of nuclear species. We already have a hint for the latter in case of the abundance of heavy nuclei (Ohnishi 1973, Arnould 1972).

Primordial nucleosynthesis is responsible for the production of light elements, and it began around 3 minutes after the Big Bang, where the universe started expanding from a very high density state dominated by radiation (Hou et al. 2017), which evolved according to the Friedman-Robertson-Walker cosmological model (Kolb and Turner 1994). At the beginning, when the temperature of the universe was higher than 10^4 GK, the radiation was composed by hadrons, leptons and photons; but the first ones started to annihilate with their respective antiparticles, giving birth to the lepton era 10^{-4} seconds after the big explosion. The universe is then dominated by leptons and this era finished around 10 seconds later with the neutrino decoupling, when the weak interaction was slower than the expansion of the universe. By that time, the temperature was of the order of Giga-Kelvins and the number of leptons strongly decreased, while the photons became predominant (Audouze and Vauclair 1980). There are two arguments favoring the Big Bang Theory; the red-shifted absorption lines emitted by the galaxies and the observation of the cosmic microwave background. Also there is a considerable consistency between calculation and observations of abundances of light elements produced in primordial nucleosynthesis. The standard primordial abundance models rely on the assumption that the nuclei follow the Boltzmann statistics, however, with this assumption it hadn't been possible to explain the observed abundance of Lithium 7. With the inclusion of temperature dependent masses (and binding energies), we plan to calculate the reaction rates and the abundance of Lithium and the other light elements at different temperatures. On the other hand, we plan to evaluate the temperature dependent screening effects in stellar nucleosynthesis with the inclusion of the new screening potential, that comes from equations such as the Thomas-Fermi equation, in the reaction rates. Electron screening effects appear in different environments such as degenerate or non-degenerate matter, dilute or dense matter at extremely high or relatively low temperatures depending on the type of nucleosynthesis involved. Indeed, the type of environment also determines the kind of statistics to be used. One of the objectives of this work is to identify the appropriate equation involved for a given environment and solve it exactly to study the effect of temperature dependent screening on reaction rates which can affect the abundance of elements.

2 Theoretical Framework

2.1 Reaction rates and nuclear abundances

2.1.1 Reaction rates

In thermonuclear reactions the kinetic energy of the nuclei is provided by the temperature of the surrounding. In a non-relativistic environment, that kinetic energy is related with the velocities classically as:

$$K_i = \frac{1}{2} m_i v_i^2$$

The probability of occurrence of a nuclear reaction depends on the relative velocities of the interacting nuclei. Assuming again that individual velocities fall into the non-relativistic regime, each of these can be described by a Maxwell-Boltzmann distribution (Iliadis 2015) and hence, the relative velocities for two nuclei with masses m_0 and m_1, are also described by the Maxwell-Boltzmann distribution (Clayton 1983) as:

$$P(v)dv = \left(\frac{m_{01}}{2\pi kT}\right)^{3/2} e^{-m_{01}/(2kT)} 4\pi v^2 dv, \tag{1}$$

where m_{01} is the reduced mass, k is the Boltzmann constant and T the surrounding temperature. This expression can be rewritten in terms of the kinetic energy of the system ($E = m_{01}v^2/2$)

$$P(v)dv = P(E)dE = \frac{2E^{1/2}}{(\pi^{1/3}kT)^{3/2}} e^{-E/kT} dE. \tag{2}$$

The reaction rate of the two nuclei in terms of the energy distribution (Iliadis 2015) is:

$$r_{01} = N_0 N_1 \left(\frac{8}{\pi m_{01}}\right)^{1/2} \frac{1}{(kT)^{3/2}} \int_0^{\infty} E\sigma(E) e^{-E/kT} dE, \tag{3}$$

where N_0 and N_1 are the number densities of species 0 and 1, respectively. $\sigma(E)$ is the cross section of the interaction (a measure of the probability that the reaction occurs). Then, for a reaction $0 + 1 \rightarrow 2 + 3$, the reaction rate per particle pair involving two particles (all of them with mass) is

$$\langle \sigma v \rangle_{01} = \left(\frac{8}{\pi m_{01}}\right)^{1/2} \frac{1}{(kT)^{3/2}} \int_0^{\infty} E_{01} \sigma_{01\rightarrow 23} e^{-E_{01}/kT} dE_{01}, \tag{4}$$

and the reverse reaction ($2 + 3 \rightarrow 0 + 1$):

$$\langle \sigma v \rangle_{23} = \left(\frac{8}{\pi m_{23}}\right)^{1/2} \frac{1}{(kT)^{3/2}} \int_0^{\infty} E_{23} \sigma_{23\rightarrow 01} e^{-E_{23}/kT} dE_{23} \tag{5}$$

We particularly are using E_{01} and E_{23} as integration variables to exploit later the relation $E_{23} - E_{01} = Q_{01\rightarrow 23}$, with E_{01} being the kinetic energy in the center of mass of 0 and 1, and E_{23} the kinetic energy in the center of mass of 2 and 3. The *reciprocity theorem* states that the forward and backward cross sections are related by the density of final states, and the number of states available for momenta between $p + dp$ is proportional to p^2 and to the statistical weight that depends on the particle's spin after the reaction (Kamal 2014). Thus, cross sections in 4 and 5 are related as:

$$\frac{\sigma_{01\to 23}}{\sigma_{23\to 01}} = \frac{(2j_2+1)(2j_3+1)p_{23}^2}{(2j_0+1)(2j_1+1)p_{01}^2} \tag{6}$$

Since $p^2 = 2mE$, we can write the former equation as:

$$\sigma_{01\to 23} = \sigma_{23\to 01}\frac{(2j_2+1)(2j_3+1)E_{23}m_{23}(1+\delta_{01})}{(2j_0+1)(2j_1+1)E_{01}m_{01}(1+\delta_{23})} \tag{7}$$

The factor $1+\delta_{ij}$ appears to take into account the effect of identical particles, which is twice the effect of different particles. Replacing $\sigma_{01\to 23}$ in 4 and dividing by equation 5 we get:

$$\frac{\langle\sigma v\rangle_{01}}{\langle\sigma v\rangle_{23}} = \frac{(2j_2+1)(2j_3+1)(1+\delta_{01})}{(2j_0+1)(2j_1+1)(1+\delta_{23})}\left(\frac{m_{23}}{m_{01}}\right)^{3/2}\frac{e^{E_{23}/kT}}{e^{E_{01}/kT}}, \tag{8}$$

but by definition, the Q-value in a nuclear reaction is the difference in the kinetic energies, then the reverse reaction can be written as:

$$\langle\sigma v\rangle_{23} = \langle\sigma v\rangle_{01}\frac{(2j_0+1)(2j_1+1)(1+\delta_{23})}{(2j_2+1)(2j_3+1)(1+\delta_{01})}\left(\frac{m_{01}}{m_{23}}\right)^{3/2} e^{-Q_{01\to 23}/kT} \tag{9}$$

The above formalism which is standard and given in more detail in text books was mentioned in order to arrive at equation 9, which we propose to modify by including a temperature dependence in the Q value. The relation is somewhat different if one of the interacting particles is massless. However, one obtains a similar exponential factor with the Q value of the reaction.

2.1.2 Nuclear abundance and its evolution

Nuclear abundance is normally measured within a given volume (number abundance) or with respect to the abundance of another nucleus (relative abundance). For instance, abundance of Lithium 7 in primordial nucleosynthesis is expressed in terms of protons. Another way to express abundances is in terms of the mass fraction. The mass fraction of a nucleus i, X_i, is the total mass of the species i in a given volume divided by the mass density, such that $\sum_i X_i = 1$. Then abundance of a species i is defined as (Iliadis 2015):

$$Y_i = \frac{X_i}{(m_i/m_u)}, \tag{10}$$

where m_i/m_u is the relative atomic mass, i.e. the mass of the species i in atomic mass units[1]. The abundance evolution of a nucleus 0 in a reaction between nuclei 0 and 1, is modeled in a straightforward way as a first order differential equation:

$$\frac{dN_0}{dt} = -N_0 N_1 \langle \sigma v \rangle_{01} \tag{11}$$

In terms of the abundance expression (equation 10), we can write 11 as:

$$\frac{dY_0}{dt} = -\rho N_A Y_0 Y_1 \langle \sigma v \rangle_{01}, \tag{12}$$

where the ρ is the mass density and N_A the Avogadro's number. The abundance evolution process is governed by creation and destruction rates associated with the reactions, and in general the processes include the weak interaction and photodisintegration among others.

$$\begin{aligned}\frac{dY_i}{dt} = &\sum_{k,l} \rho N_A Y_k Y_l \langle \sigma v \rangle_{kl \to i} + \sum_m \lambda_{\beta, m \to i} Y_m + \sum_n \lambda_{\gamma, n \to i} Y_n \\ &- \sum_o \rho N_A Y_o Y_i \langle \sigma v \rangle_{oi} - \sum_p \lambda_{\beta, i \to p} Y_i - \sum_q \lambda_{\gamma, i \to q} Y_i\end{aligned} \tag{13}$$

The plus sign refers to creation and the minus sign to destruction. Since the abundance of a species Y_i depends on the abundance of another species, say Y_j, which itself satisfies a differential equation like 13, one ends up having a set of N coupled differential equations for N number of species in an environment. To solve these coupled differential equations analytically is practically impossible and calculations

[1]Sometimes this relative atomic mass is approximated by the number of nucleons.

are usually done using standard numerical codes available for nucleosynthesis.

Abundance in nuclear statistical equilibrium in the big bang nucleosynthesis

Nuclear statistical equilibrium is reached when the timescale of the nuclear reactions is low enough compared to the expansion of the universe, which is related with a slow change in the temperature. Statistically, the equilibrium is achieved when the entropy is maximized. By definition, the entropy of a system with energy E and N nuclear species is proportional to the logarithm of the number of possible arrangements of those species that achieve a total energy E (Wallerstein et al. 1997).

According to the Boltzmann statistics we can define the grand canonical partition function for a nucleus of a species A as (D'Hoker 2012):

$$Z_g = \sum_N \frac{gV \exp(\mu N \beta)}{N! h^3} \int \exp(-\beta E) d\Gamma, \tag{14}$$

with g the statistical weight, $\beta = 1/(kT)$, V the volume, μ the chemical potential and h and k are the Planck's and Boltzmann's constants, respectively. The integration is over the six dimensional phase space. We can write the energy with a non-relativistic approximation as $E = mc^2 + p^2/2m$ and solving the integral for the six coordinates of the phase space, we have:

$$Z_g = \sum_N \left[gV \exp\left\{(\mu - mc^2)\beta\right\} \left(\frac{2\pi m}{\beta h^2}\right)^{3/2}\right]^N /N! \tag{15}$$

The quantities inside the bracket do not depend on N, thus, for our purposes they can be represented by a constant λ. The sum can be approximated by an exponential for $N > 1$ as:

$$Z_g = \sum_N \lambda^N / N! \approx e^\lambda \tag{16}$$

The statistical average of the number of nuclei of that species is given:

$$\langle N \rangle = kT \frac{d\ln(Z_g)}{d\mu}, \tag{17}$$

$\hbar$ and c equal to 1, and taking the derivative, we have:

$$\langle N \rangle = Vg \left(\frac{mkT}{2\pi}\right)^{3/2} e^{\frac{(\mu-m)}{kT}}. \tag{18}$$

If we divide both sides by the volume, we obtain the number density, n, of the species A. Chemical equilibrium is obtained when nuclear reactions occur rapidly compared to the expansion rate. In chemical equilibrium, the chemical potential of the species A(Z) is related to the neutron and proton chemical potentials (Kolb and Turner 1994) by:

$$\mu_A = Z\mu_p + (A-Z)\mu_n, \tag{19}$$

then the former equation can be expressed as:

$$e^{\mu_A/kT} = e^{Z\mu_p/kT} + e^{(A-Z)\mu_n/kT} \tag{20}$$

Using the definition of binding energy:

$$B(A,Z,N) = Zm_z + (A-Z)m_n - m(A,Z), \tag{21}$$

and since from 18 we can obtain $e^{\mu_i/kT}$ for $i = A, Z$ and $A-Z$, then equation 20 will take the following form:

$$n_A = g_A A^{3/2} 2^{-A} \left(\frac{2\pi}{m_n kT}\right)^{3(A-1)/2} n_p^Z n_n^{A-Z} e^{B(A,Z,N)/kT} \tag{22}$$

In terms of abundances, equation 22 can be written as:

$$Y_A = g_A A^{3/2} 2^{-A} \left(\frac{2\pi}{m_n kT}\right)^{3(A-1)/2} (\rho N_A)^{A-1} A^{3/2} Y_p^Z Y_n^{A-Z} e^{B(A,Z,N)/kT}, \tag{23}$$

where N_A is the Avogadro number and ρ is the density of the surroundings. The binding energy as defined in 21 depends on the mass of the nucleus. A temperature dependent mass will lead to a temperature dependent binding energy and hence an additional temperature dependence in equation 23.

2.1.3 Reactions in Primordial Nucleosynthesis

The main reactions involved in primordial nucleosynthesis are (Hou et al. 2017):

$^{1}\mathrm{H}(\mathrm{n},\gamma)^{2}\mathrm{H}$	$^{2}\mathrm{H}(\mathrm{p},\gamma)^{3}\mathrm{H}$	$^{2}\mathrm{H}(\mathrm{d},\mathrm{n})^{3}\mathrm{He}$
$^{2}\mathrm{H}(\mathrm{d},\mathrm{p})^{3}\mathrm{H}$	$^{3}\mathrm{H}(\mathrm{d},\mathrm{n})^{4}\mathrm{He}$	$^{3}\mathrm{H}(\alpha,\gamma)^{7}\mathrm{Li}$
$^{3}\mathrm{He}(\mathrm{n},\mathrm{p})^{3}\mathrm{H}$	$^{3}\mathrm{He}(\mathrm{d},\mathrm{p})^{4}\mathrm{H}$	$^{7}\mathrm{Li}(\mathrm{p},\alpha)^{4}\mathrm{He}$
$^{3}\mathrm{He}(\alpha,\gamma)^{7}\mathrm{Be}$	$^{7}\mathrm{Be}(\mathrm{n},\mathrm{p})^{7}\mathrm{Li}$	$^{3}\mathrm{H}(\mathrm{p},\gamma)^{4}\mathrm{He}$
$^{2}\mathrm{H}(\alpha,\gamma)^{6}\mathrm{Li}$	$^{6}\mathrm{Li}(\mathrm{p},\alpha)^{3}\mathrm{He}$	$^{7}\mathrm{Be}(\mathrm{n},\alpha)^{4}\mathrm{He}$
$^{7}\mathrm{Li}(\mathrm{d},\mathrm{n})2\,^{4}\mathrm{He}$	$^{7}\mathrm{Be}(\mathrm{d},\mathrm{p})2\,^{4}\mathrm{He}$	$^{2}\mathrm{H}(\mathrm{n},\gamma)^{3}\mathrm{H}$
$^{3}\mathrm{He}(\mathrm{n},\gamma)^{4}\mathrm{He}$	$^{3}\mathrm{He}(^{3}\mathrm{He},2\mathrm{p})^{4}\mathrm{He}$	$2\,^{4}\mathrm{He}(\mathrm{n},\gamma)^{9}\mathrm{Be}$
$^{6}\mathrm{Li}(\mathrm{p},\gamma)^{7}\mathrm{Be}$	$^{6}\mathrm{Li}(\mathrm{n},\gamma)^{7}\mathrm{Li}$	$^{6}\mathrm{Li}(\mathrm{n},\alpha)^{3}\mathrm{H}$
$^{7}\mathrm{Li}(\mathrm{n},\gamma)^{7}\mathrm{Li}$	$^{8}\mathrm{Li}(\mathrm{n},\gamma)^{9}\mathrm{Li}$	$^{8}\mathrm{Li}(\mathrm{p},\mathrm{n})2\,^{4}\mathrm{He}$
$^{9}\mathrm{Li}(\mathrm{p},\alpha)^{6}\mathrm{He}$	$^{9}\mathrm{Be}(\mathrm{p},\alpha)^{6}\mathrm{Li}$	$^{9}\mathrm{Be}(\mathrm{p},\mathrm{d})2\,^{4}\mathrm{He}$

The reaction rates of some of the reactions will be negligible compared to others, and probably effects of temperature in such cases will also be insignificant, but they will be taken into account.

2.2 Temperature dependence of nuclear masses

Usually, nuclear masses are treated as constants, however, it seems reasonable to expect that they are affected by the temperature in an astrophysical environment. The mass of a nucleus with Z protons and N neutrons is:

$$m(Z,N)c^2 = Zm_z c^2 + Nm_n c^2 - B(Z,N) \tag{24}$$

where m_z is the mass of the proton, m_n is the mass of a neutron and $B(Z,N)$ is the binding energy of the nucleus. There exist different approaches in literature to model the temperature dependence of the binding energy (Davidson et al. 1994, Guet et al. 1988). We will assume that the binding energy depends on the temperature, and this dependence is directly related with the excitation energy, E^*, of the nucleus[2].

$$B(Z,N,T) = B(Z,N,0) - E^* \tag{25}$$

From equations 24 and 25, we can write an expression for the mass depending on the temperature.

$$m(Z,N,T)c^2 = m(Z,N)c^2 + E^* \tag{26}$$

To get the excitation energy, we assume that the nucleus behaves as a Fermi gas and we approximate E^* by its average (Davidson et al. 1994). First we define the partition function as:

$$Z = \sum_i^{E_m} g_i \exp(-E_i^*/kT) + \int_{E_m}^{\infty} \rho(E) \exp(-E/kT) dE, \tag{27}$$

where g_i is the statistical weight defined as $j_i(j_i+1)$ and j_i the spin in the level i. $\rho(E)$ is the density of states. The right hand side has a discrete part (the sum) and a continuous part (the integral). The first one is summing over all of the known excited states of the nucleus and E_m is the highest known energy. The second one includes all the unknown energies beyond E_m. We take the density of states function for light nuclei from Couteur and Lang (1959), which has the following form:

$$\rho(E) = \exp\left(2[a(E-b)]^{1/2}\right), \tag{28}$$

[2]If the nucleus is excited, then less energy is required to break the nucleus apart.

where a is the level density parameter. We take some values of a from Murata (2001). However there are some other nuclei for which a is not given in the document; for them we made a prediction fit using Ordinary Least Square (OLS) with the information available of light nuclei. The calculations lead to the following expression:

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

We also tried combinations of Z, Z^2, A^2, AZ in the regression, but the former equations presented the least estimated error.

From statistical physics we know that the average excitation energy can be obtained in terms of the partition function as:

$$\bar{E}^* = -\frac{\partial \ln Z}{\partial \beta}, \tag{29}$$

with $\beta = 1/(kT)$. Using 28 in 27, and solving equation 29, we find the average excitation energy.

$$\bar{E}^* = \frac{\displaystyle\sum_i^{E_m} E_i^* g_i \exp(-E_i^*/kT) + \int_{E_m}^{\infty} E\rho(E)\exp(-E/kT)dE}{\displaystyle\sum_i^{E_m} g_i \exp(-E_i^*/kT) + \int_{E_m}^{\infty} \rho(E)\exp(-E/kT)dE} \tag{30}$$

The integrals will be calculated numerically using Fortran and as mentioned, the discrete part is calculated with the experimental available information.[3]

Finally, taking $E^* = \bar{E}^*$, the mass of a nucleus with Z protons and N neutrons (equations 26 and 30) is:

[3]https://www.nndc.bnl.gov/nudat2/

$$m(Z,N,T)c^2 = m(Z,N)c^2 + \frac{\sum_i^{E_m} E_i^* g_i \exp(-E_i^*/kT) + \int_{E_m}^{\infty} E\rho(E)\exp(-E/kT)dE}{\sum_i^{E_m} g_i \exp(-E_i^*/kT) + \int_{E_m}^{\infty} \rho(E)\exp(-E/kT)dE} \tag{31}$$

Preliminary calculations of temperature dependent masses and thereby the temperature dependent binding energies have been done in order to calculate the abundances in nuclear statistical equilibrium as given in equation 23. Though we do not enter into the details of these results, we would like to mention here that they hint toward the change in the lithium abundance (which has been a puzzle for some time [Yamazaki et al. 2014, Hou et al. 2017, Bertulani et al. 2018]) in the right direction. The results have motivated us to plan a modification of the existing big bang nucleosynthesis network codes to include the temperature dependent masses and hence Q-values and binding energies explicitly.

2.3 Screening in the reaction rates

The presence of electrons around the nucleus reduces the Coulomb potential generated by the nucleus, which increases the probability of an inelastic scattering with another nucleus. Screening effects using the Debye formalism (Salpeter 1954) have shown to have not significant effects on abundances in the Big Bang Nucleosynthesis (Singh and Lohiya 2015, Famiano et al. 2016, Wang et al. 2011). However there are other stellar environments where screening could have a higher impact in the reactions rates. In what follows we show how to calculate the electrostatic potential using the Thomas-Fermi equation with temperature corrections. Marshak and Bethe (1940) have shown that the Thomas-Fermi model is appropriate for red dwarf where the density is between 1000 and 100000 kg/m^3 (Aller 1950). In general, the Thomas-

Fermi model is adequate for stellar environments with a high degree of degeneracy pressure and a moderate temperature. With this, we plan to perform a more sophisticated calculation of temperature dependent electron screening for reactions in stellar environments.

2.3.1 Screening potential with direct temperature effects

Feynman et al. (1949) postulated a self-consistent Poisson-like equation with the following form:

$$\nabla^2 \Phi_{fmt} = \int d^3p FD(\Phi_{fmt}, T, p), \tag{32}$$

where FD stands for the Fermi-Dirac distribution. From this, the Thomas-Fermi and the Poisson-Boltzmann equations can be derived. In general, the Feynman-Metropolis-Teller equation can be written as (Bermudez et al. 2017):

$$\nabla^2 \Phi = \rho(r, T), \tag{33}$$

in this context $\rho(r, T)$ is the charge density associated with the particles found in the gas and its form will vary according to the astrophysical conditions.

The electrostatic potential in a degenerated gas of fermions is connected with the Thomas-Fermi function in a point r (Marshak and Bethe 1940), by:

$$\frac{Ze^2\Phi}{r} = eV + E_F, \tag{34}$$

where E_F is the Fermi energy of the electrons, r is equal to ax and $a = a_0(9\pi^2/128Z)^{1/3}$, a_0 being the first Bohr orbit for Hydrogen. Φ satisfies the asymptotic form of the generalized Thomas-Fermi equation, given by:

$$\frac{d^2\Phi}{dx} = \frac{\Phi^{3/2}}{x^{1/2}} \left[1 + \sum_n \xi_n (kTx/\Phi)^{2n} \right], \tag{35}$$

with $\xi_n = (a/Ze^2)^{2n} a_n$. The coefficients a_n will be taken from McDougall and Stoner

(1938). To solve the Thomas-Fermi equation, we will follow the work of Gilvarry (1954) where the solutions to the temperature perturbations are given in terms of quadratures. The proposed solution have the following form:

$$\Phi = \phi + \sum_n \chi_n(x)\xi_n(kT)^{2n}, \tag{36}$$

where ϕ is a solution of the Thomas-Fermi equation without a temperature perturbation. Each perturbation χ_n satisfies an inhomogeneous linear differential equation with the form:

$$\frac{d^2\chi_n}{dx^2} = \frac{3}{2}\left(\frac{\phi}{x}\right)^{1/2}\chi_n + f_n, \tag{37}$$

f_n is a function of x, ϕ, χ_i for $i = 1, 2, ..., n-1$, and it comes from equations 36 and 37. The boundary conditions are:

$$\chi_n(0) = 0 \tag{38a}$$

$$\chi_{n,b} = x_b[d\chi_n/dx]_{x=xb} \tag{38b}$$

The general solution for χ_n is:

$$\chi_n = [c_1 J_1(x) + J_{21}(f_n, x)]\left[\phi + \frac{1}{3}x\frac{d\phi}{dx}\right] \tag{39}$$

The constant c_1 can be regarded as the initial slope of the solution and is obtained with the initial conditions, equations 38a and 38b (Gilvarry 1954). The J's are written in terms of integrals with x and f_n dependance[4]. They have the following

[4]Directly they depend on ϕ, but ϕ is a function of x.

form:

$$J_1(x) = \int_0^x \left(\phi + \frac{1}{3}z\frac{d\phi}{dz}\right)^{-2} dz \tag{40a}$$

$$J_2(f_n, x) = \int_0^x f_n \left(\phi + \frac{1}{3}z\frac{d\phi}{dz}\right) dz \tag{40b}$$

$$J_{12}(f_n, x) = \int_0^x J_1(z) f_n \left(\phi + \frac{1}{3}z\frac{d\phi}{dz}\right) dz \tag{40c}$$

$$J_{21}(f_n, x) = \int_0^x J_2(f_n, z) \left(\phi + \frac{1}{3}z\frac{d\phi}{dz}\right)^{-2} dz \tag{40d}$$

The four identities also have to satisfy:

$$J_1(x)J_2(f_n, x) = J_{12}(f_n, x) + J_{21}(f_n, x) \tag{41}$$

The first three values of f_n are:

$$f_1 = \frac{x^{3/2}}{\phi^{1/2}} \tag{42a}$$

$$f_2 = \frac{1}{x\phi}^{1/2} \left[\frac{x^4}{\phi^2} - \frac{a_1^2}{a_2}\left(\frac{1}{2}\frac{x^2}{\phi}\chi_1 - \frac{3}{8}\chi_1^2\right)\right] \tag{42b}$$

$$f_3 = \frac{1}{x\phi}^{1/2} \left[\frac{x^6}{\phi^4} - \frac{a_1^3}{a_3}\left(\frac{3}{8}\frac{x^2}{\phi^2}\chi_1^2 - \frac{1}{16}\chi_1^3\right) - \frac{a_1 a_2}{a_3}\left(\frac{5}{2}\frac{x^4}{\phi^3}\chi_1 - \frac{1}{2}\frac{x^2}{\phi}\chi_2 - \frac{3}{4}\chi_1\chi_2\right)\right] \tag{42c}$$

The integrals will be solved numerically. With the values of the J's we can calculate χ_n using equation 39. Then we have a solution for the Thomas-Fermi function, Φ, and finally for the electrostatic potential in equation 34.

Part of this work is to explore other astrophysical conditions where the gas surrounding the nuclei has different characteristics and the potential would be described by different equations as shown in Bermudez et al. (2017). As we mentioned, the case presented in this section was for degenerated matter, where the density is high enough for a given temperature. For dilute matter the equation describing the potential is a generalization of the Poisson-Boltzmann equation, and it can be approximated to the Debye-Hückel equation as shown in Bermudez et al. (2017).

$$-\nabla^2\Phi + \frac{2e^2 n_0}{T}\Phi = \rho(r), \tag{43}$$

with n_0 the concentration of particles. Also it can be assumed that the statistics of the species inside the gas follows a Tsallis distribution instead of a Maxwell-Boltzmann distribution (Hou et al. 2017), which is useful for high density environments like neutron stars. With that assumption we can obtain the following differential equation for the potential (Bermudez et al. 2017):

$$\frac{d^2\Phi}{dx^2} = \frac{\Phi^{3/2}}{\sqrt{x}}\left(1 + \chi_1\frac{Tx}{\Phi} + \chi_2\frac{T^2x^2}{\Phi^2}\right), \tag{44}$$

with χ_1 and χ_2 given in Bermudez et al. (2017). Notice the similarities of equations 35 and 44, but now the equation is including odd terms of the temperature, while before it was only even terms.

2.4 Modified reaction rates

The screening effect comes into play through the cross section. Equation 4 shows the reaction rate depending on $\sigma_{01\to 23}$, or more generally on $\sigma(E)$. The cross section is given by:

$$\sigma(E) = \frac{1}{E}S(E)P, \tag{45}$$

with P the transmission probability and S(E) the astrophysical S-factor. The former, within the semi-classical WKB approximation is given by:

$$P(\Phi) \approx \exp\left(-\frac{2}{\hbar}\sqrt{2m_{01}}\int_0^{R_c}\sqrt{V(r) - E}dr\right) \tag{46}$$

R_c is the distance to the classical turning point. Notice that $V(r)$ is connected to Φ according to the equation 34. The S-factor can be expressed as a Taylor series around $E = 0$ (Iliadis 2015) as:

$$S(E) \approx S(0) + S'(0)E \tag{47}$$

$S(0)$ and $S'(0)$ are empirical determined constants, and may vary according to the reaction (Caughlan and Fowler 1962). Thus, the reaction rate per particle pair expression is:

$$\langle \sigma v \rangle_{01} = \left(\frac{8}{\pi m_{01}(T)} \right)^{1/2} \frac{1}{(kT)^{3/2}} \int_0^\infty P(\Phi, E) S(E) e^{-E_{01}/kT} dE \tag{48}$$

Here we are also taking into account the temperature effect on the nuclear masses (equation 31). There is an additional temperature effect on the reaction rate, and is more related with the reverse reaction. From the reciprocity theorem (equation 9), the reverse reaction depends on the Q-value, that by definition is also a function of the masses, as follows:

$$Q = (m_0 + m_1 - m_2 - m_3)c^2 \tag{49}$$

With the new masses, it is expected that we will have also a modification in the Q-values of the reaction, changing at the same time the destruction rates associated with the reverse reaction. For the abundances in the Big Bang Nucleosynthesis we will take into account only the modifications in the masses and Q-values into the reaction rates, whereas in other stellar environments we will include also the temperature-screening correction. In order to compare the obtained results, we will calculate as well abundances in nuclear statistical equilibrium using equation 23.

3 Objectives

3.1 General Objective

Investigate the so far unexplored effects that the surrounding temperature has on the reaction rates involved in the nucleosynthesis process and how they affect the abundances of several nuclei.

3.2 Specific Objectives

- Study the temperature dependence of nuclear masses in the Big Bang and other stellar environments using the formalism mentioned in this proposal.
- Study the temperature dependence in the electron screening calculations within a relativistic Thomas Fermi model and compare the results with the simpler calculations existing in literature.
- Calculate new reaction rates taking into account the temperature effects associated to masses and electron screening as mentioned above.
- Modify nucleosynthesis codes with the adjusted reaction rates and obtain new nuclear abundances.
- Compare the results obtained with calculations of previous works.

4 Methodology

We will start with reviewing more literature to check for updates in approaches to the proposed problems and equations. After that, we will calculate average excitation energies for the nuclei involved in nucleosynthesis in the Big Bang. With those energies we will calculate nuclear masses depending on the temperature and the Q-values, as well as the reactions of light nuclei within the formalism mentioned in this proposal. Then we plan to obtain the abundances using available codes on big bang nucleosynthesis, like the one of Kawano (1988). The other part of the work consists in finding the Thomas-Fermi function to obtain the screening potential with a direct temperature effect as shown above, and to study different equations of the Feynman-Metropolis-Teller type that are a appropriated for given astrophysical environments. With the screening potential, and with the new masses and Q-values, we shall calculate the corrections in the reaction rates. Many of the calculations will have to be done numerically so we will use standard numerical methods and the help of softwares like Fortran and Stata. There will be regular meetings with the supervisor to discuss the progress and also a constant review of previous investigations to compare the obtained results.

5 Ethical considerations

We will construct the body of this research by developing a formalism and performing calculations using available literature on the subject. We shall use nucleosynthesis codes which are publicly available on academic web sites and modify them to obtain our results. External data is required as well for comparisons of the results in this investigation with available calculations. We will refer to the authors who developed the data and models used to create and compare the calculations of this thesis document and we will give the appropriate citations of the publicly available nucleosynthesis codes. There is no conflict of interest with this research, reason why this investigation doesn't have to be sent to the Ethical Committee of the Faculty of Science.

6 Timeline

Activity	**Months**
Additional literature review	2 months
Calculation of average excitation energies and	3 months

temperature dependent nuclear masses	
Calculation of the Thomas-Fermi function and screening potential	4 months
Review other equations relevant for different astrophysical environments and the screening corrections with the selected equations	6 months
Calculation of the reaction rates with the adjusted potentials, masses and Q-values	4 months
Calculation of abundances with the BBN-code	5 months
Analysis of results	3 months
Preparation of the document and thesis presentation	3 months

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