Applications of q-Statistics in Big Bang Nucleosynthesis

A Project Report Submitted for the degree of

 $\begin{array}{c} \text{Bachelor of Technology} \\ \text{ } \\ \text{in} \\ \text{Engineering Physics} \end{array}$

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Candidate's Declaration

I hereby declare that the work, which is being presented in this report entitled "Applications of q-Statistics in Big Bang Nucleosynthesis" and submitted in partial fulfilment of the requirements of the degree of Bachelor of Technology in Engineering Physics as an authentic record of my own work carried out during the period of August 2021 to April 2022 under the supervision of Dr. Rajdeep Chatterjee, Department of Physics, IIT Roorkee. The matter contained in this report has not been submitted by me for the award of any other degree in the institute or any other Institute/University.

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Certificate

This is to certify that the project entitled "Applications of q-Statistics in Big Bang Nucleosynthesis" is a bonafide work carried out by Manish Prasad, B.Tech final year student IIT Roorkee, in the partial fulfilment for the requirements of the award of the degree Bachelor of Technology in Engineering Physics under my guidance.

Rajdeep Chatterjee

Professor Department of Physics Indian Institute of Technology Roorkee

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1 Abstract

This work describes the use of Tsallis non extensive statistics to calculate the abundances of light elements during big bang nucleosynthesis. The theory of Tsallis entropy, and it's impact on the Maxwell Boltzmann distribution was studied. Then, the new reaction rates were calculated using the non extensive statistics. The abundances of light nuclei were calculated using a BBN code and the impact of this q-parameter and the drawbacks of this model were discussed.

2 q-Logarithm and q-Exponential Functions

Consider the function $\frac{dy}{dx} = y^q$. The solution of this differential equation is:

$$y = [1 + (1 - q)x]^{1/(1-q)}$$

And the inverse is:

$$y = \frac{x^{1-q} - 1}{1 - q}$$

We can define these two solutions differently in the form of q-logarithm and q-exponential functions:

$$\ln_q x = \frac{x^{1-q} - 1}{1 - q} \qquad (x > 0; \ \ln_1 x = \ln x)$$
 (2.1)

$$e_q x = [1 + (1-q)x]^{1/(1-q)}$$
 $(e_q^x = e^x)$ (2.2)

We can see that as $q \to 1$, $\lim_{q \to 1} \ln_q x = \ln x$ and $\lim_{q \to 1} e_q^x = e^x$. We can also observe the following property:

$$\ln_q(x_a x_b) = \ln_q x_a + \ln_q x_b + (1 - q) \ln_q(x_a) \ln_q(x_b)$$
 (2.3)

More information about this can be found in Chapter 3 of [15] and some important properties of the q-logarithm and q-exponential can be found in [18]. The graphs of the q-logarithm and q-exponential functions look like:

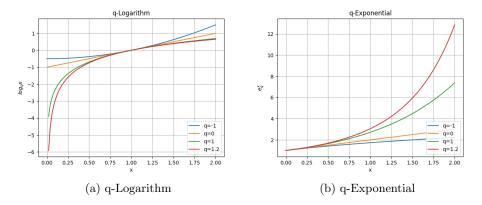


Figure 1: Graphs of q-Logarithm and q-Exponential plotted using Python

3 Tsallis Entropy

3.1 Boltzmann-Gibbs Entropy

The Boltzmann–Gibbs (BG) entropy is given by (for a set of W discrete states):

$$S_{BG} = -k \sum_{i=1}^{W} p_i \ln p_i$$
 ; where $\sum_{i=1}^{W} p_i = 1$ (3.1)

Here k is a positive constant which is the Boltzmann constant k_B . For the case of equal probabilities (i.e., $pi = 1/W, \forall i$), Eq.3.1 becomes:

$$S_{BG} = k \ln W \tag{3.2}$$

We can observe the following property. If we compose two independent systems A and B (with numbers of states denoted by W_A and W_B respectively), such that the joint probabilities factorize, $p_{ij}^{A+B} = p_i^A p_j^B(\forall (i,j))$ and $W = W_A W_B$, then the entropy $S_B G$ is additive. That is:

$$S_{BG}(A+B) = S_{BG}(A) + S_{BG}(B)$$
 (3.3)

For a canonical system in thermal equilibrium at temperature T and its mean energy U, the BG statistical mechanics yields:

$$\sum_{i=1}^{W} p_i E_i = U \tag{3.4}$$

$$p_i = \frac{e^{-\beta E_i}}{Z_{BG}} \tag{3.5}$$

where

$$\beta = \frac{1}{kT} \tag{3.6}$$

$$Z_{BG} = \sum_{j=1}^{W} e^{-\beta E_j} \tag{3.7}$$

where E_i denotes the energy spectrum and Z_{BG} is the partition function of the system.

Equations (3.1) and (3.5) are the landmarks of BG statistical mechanics. and are successfully used in physics, mathematics, computer sciences, engineering, chemistry, etc.

But using the definitions in Chapter 1, Tsallis has generalized the BG statistics as a particular case of a more generalized distribution that has applications in many complex systems. For some systems, BG statistics becomes inefficiently applicable, and a generalization of the BG Statistical Mechanics proves to be helpful.

3.2 Non-Additive Entropy

Tsallis proposed the following generalization for 3.1

$$S_q = k_b \ln_q W \tag{3.8}$$

Using the definition in (2.1), we get:

$$S_q = k_b \frac{1 - \sum_{i=1}^W p_i^q}{q - 1} \tag{3.9}$$

where q is a parameter quantifying the degree of non-extensivity. We can see the variation of S_q with W for different values of q in Figure 2. Notice, for q=1, the figure corresponds to the BG Entropy.

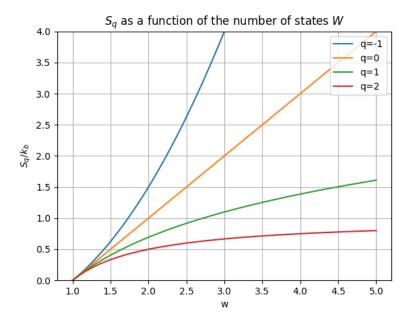


Figure 2: Equiprobability entropy Sq as a function of the number of states W, for some values of q

The property demonstrated in (3.3) now becomes:

$$S_q(A+B) = S_q(A) + S_q(B) + (1-q)S_q(A)S_q(B)$$
(3.10)

For the non-extensive scenario, we need to extremize S_q with the constraints $\sum_{j=1}^W p_i = 1$ and $\sum_{j=1}^W p_i \varepsilon_i = U_q$. This can be done using Lagrange Multipliers. This is solved in detail in [14] and we get the following results:

$$p_{i} = \frac{[1 - \beta(q - 1)\varepsilon_{i}]^{1/q - 1}}{Z_{q}}$$

$$= \frac{[1 + \beta(1 - q)\varepsilon_{i}]^{-1/1 - q}}{Z_{q}}$$

$$= \frac{e_{q}^{-\beta\varepsilon_{i}}}{Z_{q}}$$
(3.11)

where $\beta = 1/k_bT$ and:

$$Z_q = \sum_{i=1}^{W} [1 - \beta(q-1)\varepsilon_i]^{1/q-1} = \sum_{i=1}^{W} e_q^{-\beta}$$
 (3.12)

For $q \to 1$ we recover 3.5 and 3.7

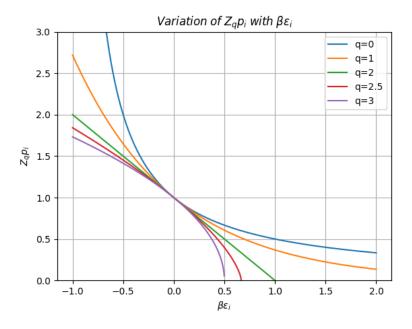


Figure 3: Variation of $Z_q p_i$ with $\beta \varepsilon_i$

From the Figure 3, we can see that when q > 1, we have a cutoff at:

$$\beta \varepsilon_i = 1/(q-1) \tag{3.13}$$

The equation 3.13 will be useful during the discussion in Chapter 5

4 Applications of Non-Extensive Statistics

A brief introduction to Non extensive statistics is provided in [16]. Non-extensive statistics has a wide range of applications (Chapter 7 [15]) in many fields like physics, chemistry, economics, computer sciences, biosciences, linguistics, etc. Following are three specific applications of q-statistics:

- Lithium Problem: Big-bang nucleosynthesis (BBN) describes the production of the lightest nuclides such as elements like H, He, Li, and Be during the first seconds of cosmic time. But, the current theory overestimates the abundance of ${}^{7}Li$. And Tsallis statistics can be helpful in solving this.
- Cryptocurrency: In [13], a study of nonextensive behavior of daily price changes for cryptocurrencies like Bitcoin has been done, from 2013 until 2017. Their results strongly indicate that the cryptocurrency market represents a state whose physics can be described by nonextensive statistical mechanics.
- Astrophysics: Temperature Fluctuations of the CMBR: In the study of CMBR (Cosmic Microwave Background Radiation), q-Gaussians are used in astrophysics and they are called κ -distributions [7], and equations are identical to Equation 2.2.

5 One Particle Maxwell Boltzmann Distribution and Tsallis Distribution

The Maxwell Boltzmann distribution is given by:

$$f_{MB}(v) = \left(\frac{m}{2\pi k_B T}\right)^{3/2} exp\left(-E/k_B T\right)$$
 (5.1)

And the Tsallis distribution is given by:

$$f_q(v) = B_q \left(\frac{m}{2\pi k_B T}\right)^{3/2} \left[1 - (q-1)\frac{E}{k_B T}\right]^{1/q-1}$$
 (5.2)

Where B_q is a normalization constant determined from the requirement $\int f_q(v_i)dv_i = 1$ and is given by:

$$B_q = (q-1)^{1/2} \left(\frac{3q-1}{2}\right) \left(\frac{1+q}{2}\right) \frac{\Gamma(\frac{1}{2} + \frac{1}{q-1})}{\Gamma(\frac{1}{q-1})} \left[\frac{m}{2\pi k_B T}\right]^{3/2}$$
 (5.3)

Derivation is given in [11] and furthur reading is provided in [6]. We can further see that from the Equation (3.13), there would be a cutoff for the Tsallis distribution. In the following figure 4, for q=1.2 there will be a cutoff at:

 $\frac{E}{k_b T} = \frac{1}{q - 1} = \frac{1}{1.2 - 1} = 5 \tag{5.4}$

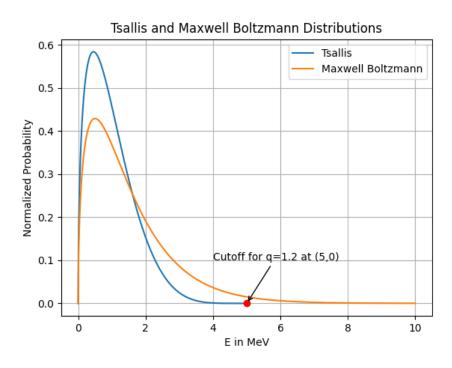


Figure 4: Tsallis distribution (at q=1.2) and M-B distribution functions with $k_BT=1 MeV$

6 Relative Velocity Distributions

A detailed derivation of all the equations in this section is given in [6]. To derive the relative velocity distributions, the three conditions need to be satisfied are:

- 1. Each nucleus is described by a non-Maxwell-Boltzmann velocity distribution
- 2. Conservation of momentum
- 3. Conservation of energy

For a two particle system, let m_i be the masses and v_i be the velocity vector of species i = 1 and 2. In the Center of Mass system, the total mass is M, the reduced mass is μ and \mathbf{v} is the relative velocity:

$$M = m_1 + m_2
\mu = \frac{m_1 m_2}{m_1 + m_2}
\mathbf{v} = \mathbf{v_1} - \mathbf{v_2}$$
(6.1)

And the momentum and energy conservations lead to:

$$V = \frac{m_1 v_1 + m_2 v_2}{m_1 + m_2} \tag{6.2}$$

$$m_1 v_1^2 + m_2 v_2^2 = MV^2 + \mu v^2$$
(6.3)

Hence, the distribution function of the relative velocity v is given by:

$$f^{rel}(oldsymbol{v}) = \int doldsymbol{V} \left[f(oldsymbol{v_1}) f(oldsymbol{v_2})
ight]_v$$

Where the term in brackets with the subscript \mathbf{v} is estimated for a fixed \mathbf{v} .

6.1 Maxwell Boltzmann

The CM distribution function of the relative velocity for the case of MB statistics has the same form as that of the individual particle distribution function (5.1):

$$f_M^{rel}(\mathbf{v}) = \frac{\mu^{3/2}}{(2\pi k_B T)^{3/2}} exp\left[-\frac{\mu v^2}{2k_B T}\right]$$
(6.4)

6.2 Tsallis Distribution

The Tsallis distribution function of the relative velocity is given by:

$$f_q^{rel}(oldsymbol{v}) = \int doldsymbol{V} \left[f_q(oldsymbol{v_1}) f_q(oldsymbol{v_2})
ight]_v$$

The ranges of V and v are calculated using (3.13):

$$m_i v_i^2 \le \frac{2k_B T}{q - 1} \tag{6.5}$$

Hence the ranges of V and v are:

$$0 \le V \le \sqrt{\frac{2k_B T}{q - 1}} \frac{\sqrt{m_1} - \sqrt{m_2}}{M} \tag{6.6}$$

$$0 \le v \le v_{1,max} + v_{2,max} = \sqrt{\frac{2k_BT}{q-1}} \left(\frac{1}{\sqrt{m_1}} + \frac{1}{\sqrt{m_2}} \right)$$
 (6.7)

Hence the distribution function becomes:

$$f_q^{rel}(v) = 2\pi \int_{-1}^1 d\cos\theta \int_0^{V_{max}} V^2 dV f_q(\mathbf{v_1}) f_q(\mathbf{v_2})$$

$$= 2\pi B_q^2 \frac{(m_1 m_2)^{3/2}}{(2\pi k_B T)^{3/2}} \int_{-1}^1 d\cos\theta \int_0^{V_{max}} V^2 dV I_q(V, \cos\theta; m_1, m_2, T, v)$$
(6.8)

Where the function I_q is given by:

$$I_{q}(V,\cos\theta;m_{1},m_{2},T,v) = \begin{cases} = \left[1 - (q-1)\frac{m_{1}v_{1}^{2}}{2k_{B}T}\right]^{1/(q-1)} \left[1 - (q-1)\frac{m_{2}v_{2}^{2}}{2k_{B}T}\right]^{1/(q-1)} \\ v_{1} \leq v_{1,max} \ and \ v_{2} \leq v_{2,max} \\ = 0 \quad (otherwise) \end{cases}$$

$$(6.9)$$

And:

$$v_1^2 = V^2 + 2\frac{m_2}{M}Vv\cos\theta + \frac{m_2^2}{M^2}v^2$$
 (6.10)

$$v_2^2 = V^2 - 2\frac{m_1}{M}Vv\cos\theta + \frac{m_1^2}{M^2}v^2$$
 (6.11)

The MB distribution $v_{th}^3 f_{MB}^{rel}(v)$ depends only E/T for a fixed q. The Tsallis distribution $v_{th}^3 f_q^{rel}(v)$ depends on the nuclear masses as well as E/T for a fixed q. This is one of the important differences from MB statistics

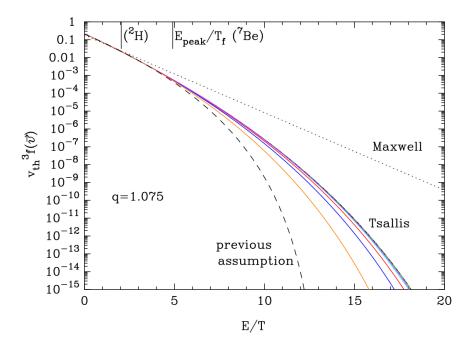


Figure 5: Normalized distributions for the center of mass energy E for q = 1.075. The dashed line is the one-particle Tsallis distribution. The dotted line corresponds to the MB distribution. The other line in between are for Tsallis statistics with (A1, A2) = (1, 1), (2, 2), (4, 3), (3, 2), (2, 1), (3, 1), and (7, 1) from top to bottom. The graph is taken from [6]

7 q-Deformed Planck Distribution

The q-Deformed Planck Distribution equation was derived in [15]. The following equations are the normal Planck distribution and the q-deformed distribution.

$$N_{\gamma}(E_{\gamma}) = \frac{8\pi}{(hc)^{3}} \frac{E_{\gamma}^{2}}{e^{E_{\gamma}/k_{B}T} - 1} dE_{\gamma}$$

$$N_{q}(E_{\gamma}) = \frac{8\pi}{(hc)^{3}} \frac{E_{\gamma}^{2}}{e^{E_{\gamma}/k_{B}T} - 1} (1 - e^{-x})^{q-1} \left\{ 1 + (1 - q)x \left[\frac{1 + e^{-x}}{1 - e^{-x}} - \frac{x}{2} \frac{1 + 3e^{-x}}{(1 - e^{-x})^{2}} \right] \right\} dE_{\gamma}$$

$$(7.2)$$

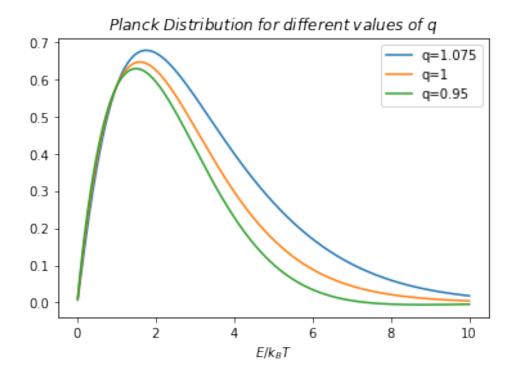


Figure 6: q-Deformed Planck Distribution

8 Reaction Rates

8.1 Charged particle reaction rate

For a charged particle reaction: $1+2 \rightarrow 3+4$, the reaction rate is given by:

$$r_{12} = N_1 N_2 \langle \sigma(v) v \rangle$$

Where v is relative velocity of the particles 1 and 2, N_1 and N_2 are the number of particles of 1 and 2 per unit volume, σ is the cross section, and $\langle \sigma v \rangle$ is the average reaction rate per particle pair. Since the particles will have a velocity distribution, in order to calculate $\langle \sigma v \rangle$, we have to integrate it over a velocity distribution.

$$\langle \sigma v \rangle = \int f^{rel}(\boldsymbol{v}) v \sigma(v) dv$$

The relation between $\sigma(E)$ and S(E) is:

$$\sigma(E) = \frac{1}{E}S(E)e^{-2\pi\eta} \tag{8.1}$$

Where $e^{-2\pi\eta}$ is the Gamow factor which gives the tunneling probability, and η is Sommerfeld parameter. For the Maxwell Boltzmann distribution, the rate equation becomes:

$$\langle \sigma v \rangle = \left(\frac{8}{\pi \mu}\right)^{1/2} \frac{1}{(k_B T)^{3/2}} \int e^{-2\pi \eta} S(E) f_q^{rel}(E) dE \tag{8.2}$$

A detailed derivation is given in Chapter 3 of [5]. And the rate equation for the Tsallis Distribution becomes:

$$\langle \sigma v \rangle = \int f_q^{rel}(\mathbf{v}) v \sigma(v) dv$$
 (8.3)

The integrand in these equations is called the Gamow function. The Gamow peak represents the which most of the nuclear reactions occur. The width of the Gamow function gives the strength of Coulomb barrier.

9 S-Factors and Reaction Rates

The best fitting curve for the S-Factors are given in [10]. The methodology of [1] and [4] was followed. The following figures are the S-factors and the Reaction rates for five of the reactions that are of primary importance to calculate Lithium abundance (See section 10)

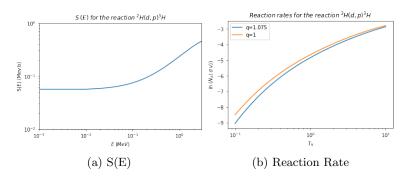


Figure 7: S(E) and Reaction Rate for d(d, p)t

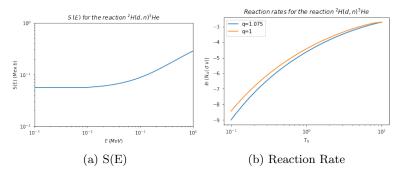


Figure 8: S(E) and Reaction Rate for $d(d,n)^3He$

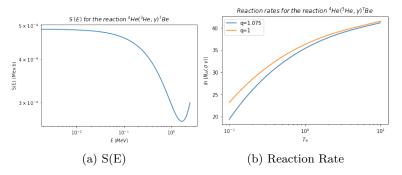


Figure 9: S(E) and Reaction Rate for $^4He(^3He,\gamma)^7Be$

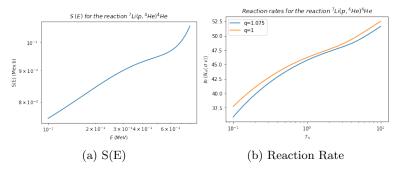


Figure 10: S(E) and Reaction Rate for $^7Li(p,^4He)^4He$

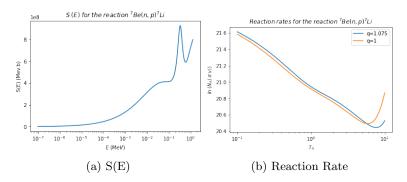


Figure 11: S(E) and Reaction Rate for ${}^{7}Be(n,p){}^{7}Li$

10 Lithium Problem

The generally accepted prediction for Lithium abundance is the one in [3] that reports ${}^{7}Li/H = (4.68 \pm 0.67)10^{-10}$, which is about 3 times greater than the widely accepted central value of observations, ${}^{7}Li/H = (1.58 \pm 0.30)10^{-10}$ ([9]). The figure 12 shows a simplified network of reactions relevant for BBN and the reactions. The actual full network goes beyond these 12 reactions, but these reactions are the most important for calculating the Lithium abundance. The full reaction network involves 30 reactions in total with nuclei of $A \leq 9$. The thermonuclear forward rates for 11 reactions of primary importance ([12],[6]) in the primordial light-element nucleosynthesis have been considered to calculate the abundances. Also, this makes it computationally less expensive.

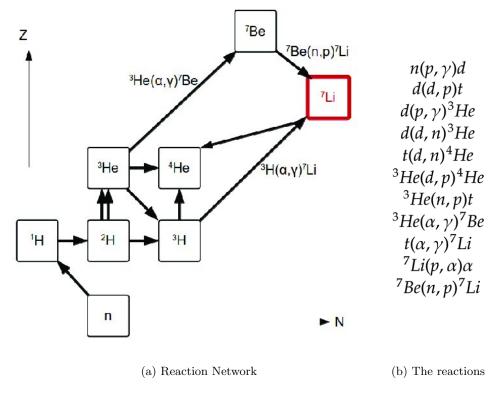


Figure 12: Simplified reaction network showing reactions forming 7 Li during the Big Bang adapted from [2]

11 Big Bang Nucleosynthesis code

The [17] package was used to run the Big Bang Nucleosynthesis (BBN) code. The project description is available at: https://pypi.org/project/BBN/#description, and the files can be found at the author's GitHub page: https://github.com/tt-nakamura/BBN. The BBN code uses the best fitting curve of the reaction rates as a function of T9 (10⁹ Kelvin) and the reaction rates are taken from [12]. This code only uses the 12 reactions that that are given in Figure 12.

11.1 Getting the best fit Curve for the rate with q-statistics

Let us consider the reaction $d(d, n)^3 He$ for demonstrating the procedure. The best fit curve for the reaction rate as given in [12], is:

$$Rate\ (cm^3s^{-1}mole^{-1}) = 3.95 \times 10^8 T_9^{-2/3} \times \exp(-4.259/T_9^{1/3}) \times (1.0 + 0.098 T_9^{1/3} + 0.765 T_9^{2/3} + 0.525 T_9 + 9.61 \times 10^{-3} T_9^{4/3} + 0.0167 T_9^{5/3})$$

$$(11.1)$$

Figure 13 shows the reaction rates for the reaction $d(d,n)^3He$. The blue graph corresponds to Equation 11.1. The orange and green graphs are the ones from Figure 8 (The graphs are not in the logarithmic scale in Figure 13)

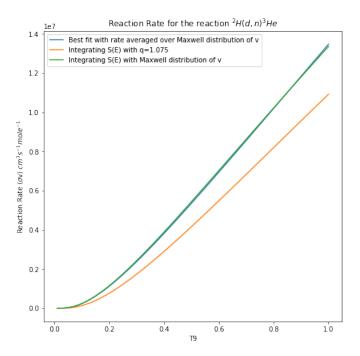


Figure 13: Reaction Rate for $d(d, n)^3 He$

To find the best fit curve for the graph with q-statistics, we need to find an expression to model the difference between the equation 11.1 and the q graph.

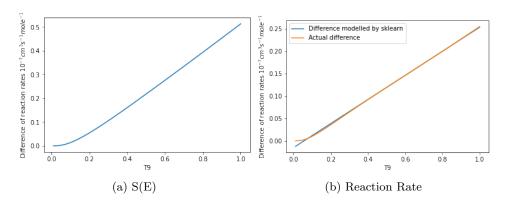


Figure 14: Difference of reaction rates and using scikit-learn to get an equation for that difference

From the library scikit-learn [8] which provides tools for data analysis, I have used LinearRegression from sklearn.linear_model, and PolynomialFeatures from sklearn.preprocessing, to get the best fit curve. Thus, equation 11.1 becomes:

$$Rate\ (cm^3s^{-1}mole^{-1}) = 3.95 \times 10^8 T_9^{-2/3} \times \exp(-4.259/T_9^{1/3}) \times (1.0 + 0.098 T_9^{1/3} + 0.765 T_9^{2/3} + 0.525 T_9 + 9.61 \times 10^{-3} T_9^{4/3} + 0.0167 T_9^{5/3}) + (-0.0150250800 + 0.268885978 \times T_9) \times 10^7$$

$$(11.2)$$

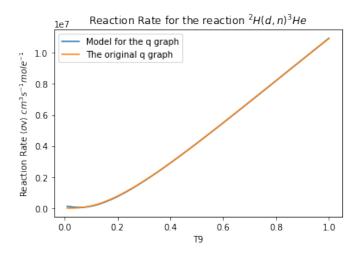


Figure 15: Model of the q graph using scikit-learn

In the figure 15, the modelled graph coincides with the original q graph. We can use this new reaction rate equation in the BBN code. This method was to all the other important reactions discussed before in 10

11.2 Abundance Curves

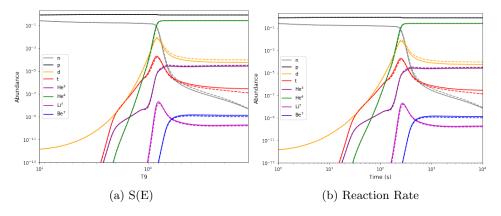


Figure 16: Abundance curves as a function of Temperature in figure (a) and Time in figure (b). The solid lines correspond to the MB statistics, and the dotted lines correspond to the Tsallis statistics

	MB BBN	q BBN	Observation	% Difference
$^4He/H$	0.249	0.2476	0.2561 ± 0.0108	-3.319%
D/H	4.192	4.3754	$3.02 \pm 0.23 (\times 10^{-5})$	38.8%
$^3He/H$	0.98	1.1793	$(1.1 \pm 0.2)(\times 10^{-5})$	7.2%
$^7Li/H$	4.39	3.7221	$(1.58 \pm 0.31)(\times 10^{-10})$	15.214%

The observation values in the above table are taken from [4]. From the above table, we can see that this q BBN code follows the trend of [1]. The paper [1] uses the value of q=0.5 and q=2, whereas this code uses the value q=1.075. Due to computational limitations, the code incorporates only the forward reactions. We can observe that although the Lithium abundance has decreased, the deuterium abundance has worsened which is consistent with the results in [6]. The implications of this are discussed in the next section.

11.3 Drawbacks of this code

The reverse reaction rates were not considered due to computational limitations. Although, their affects are more significant at higher temperatures, they still need to be considered for more accurate results.

The Deuterium abundance increases and the 7Li abundance decreases with the introduction of the q parameter, which is consistent with [6]. This could imply that there is an additional deuterium destruction mechanism. Also, the reduction in the Lithium abundance is still not enough to predict the observed values. But the predictions would be enhanced by adding the reverse reaction rates and considering even more reactions than the ones considered in this project.

11.4 Future Outlook

- 1. To calculate the abundances with the reverse reaction rates.
- 2. To study the impact of the θ parameter that was discussed in subsection 6.2. Some work on this has been done in [6].
- 3. To study the effects of non-extensive statistics in other astrophysics fields as it might offer new perspectives of nucleosynthesis.

12 Conclusion

In this project, the framework of Tsallis non-extensive statistics is used to describe the velocity distribution of nucleons. By adding a non-extensive parameter (q), the abundances of primordial abundances of light nuclei are in better agreement with the observed values. The predictions can be improved by using a more vast code that includes additional reactions along with their reverse reaction rates, where all the rates are calculated in the Tsallis framework. But even with the limitations of this project, we can observe that the Lithium abundances are better predicted in this non extensive framework and this might be a possible solution to the Lithium problem.

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