

ATOMIC PARTITION FUNCTION FOR STELLAR ATMOSPHERES AND PLASMA DIAGNOSTICS

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ABSTRACT

A new approximate partition function is derived as a function of temperature and total number density of particles in the given system, and three adjustable parameters. The derivation assumes that we can simulate the calculations of the partition function for hydrogen by means of averages of the energies and sums of the statistical weights. We present the procedure and mathematical process to obtain an approximate analytic function and its derivatives that depend on those parameters. The comparisons with other calculations reported in the literature show good agreement. The free parameters of this function are calculated and given in a table for all the ions of the first 20 atomic species.

Key words: atomic processes – equation of state – plasmas – stars: atmospheres

1. INTRODUCTION

The partition function was defined by Boltzmann as the sum over all the possible energy states that an atom can have and is represented by

$$U = \sum_{n=1}^{\infty} g_{nj} e^{-\frac{E_{nj}}{k_B T}}, \quad (1)$$

where g_{nj} is the statistical weight, E_{nj} is the excitation energy of the state n for the state of ionization j of the chemical element k , k_B is the Boltzmann constant, and T is the temperature of the thermodynamic system. In reality, n represents the electron configurations, the enumeration of the values of n and l , the principal and angular momentum quantum numbers, respectively, for all the electrons of an atom, including the multiple excited states, in the case of complex atoms. The partition function is useful in the calculation of the equation of state for stellar atmospheres and interiors as well as for plasma diagnostics through the Saha equation or through the free energy of Helmholtz for more sophisticated methods to calculate the thermodynamic parameters useful in many applications. The partition function diverges for isolated atoms due to the existence of an infinite number of available energy states. For atoms embedded in a system of particles the number of energy states in the atoms is finite due to the physical interactions among the particles; therefore, the partition function can be numerically evaluated. In this work, we are interested in finding the partition function for atoms and ions in a partially ionized perfect gas in thermodynamic equilibrium. In the calculation of the thermodynamic properties of a gaseous system, it is necessary to know the partition function for each chemical species in its different states of ionization in order to determine the populations and other thermodynamic coefficients in stellar atmospheres and plasmas. Traditionally, the sum that defines the partition function is evaluated, taking into account very few terms of the power series expansion of the exponentials. In general, the numerical results are presented in tables of the partition function for some temperatures and electronic densities and is necessary to make interpolations when they are required in the given applications. Those results do not produce compact analytic functions necessary for the repetitive calculations required in model atmospheres and plasma diagnostics. In this work, we obtain a compact analytic partition function that is easy to use in any numerical application. In what follows, we present

in Section 2 the assumptions and mathematical procedure to find the approximate partition function and its derivatives. Section 3 presents the comparisons of the results obtained with the derived partition function with other methods and calculations. The tables obtained for the free parameters necessary to calculate the partition functions for 20 elements and their ions are explained in Section 4. Finally, in Section 5 the conclusions and discussions are presented.

2. MATHEMATICAL PROCEDURE

Following Unsöld (1948), we should split the sum in Equation (1) into two parts; in our case, we divide it into three parts for simplicity as

$$U = g_{1jk} e^{-\frac{E_{1jk}}{k_B T}} + \sum_{n=2}^{n'} g_{nj} e^{-\frac{E_{nj}}{k_B T}} + \sum_{n=n'}^{n^*} g_{nj} e^{-\frac{E_{nj}}{k_B T}}, \quad (2)$$

where the first sum is over the lowest energy states up to n' and the last one is from n' to n^* , the last remaining energy state in the atom due to the interaction of the atom with the other particles in the system. The atomic shells in hydrogen are composed of energy states that are degenerate in energy therefore the summation in Equation (1) is carried directly up to the maximum energy state available to the atoms. The procedure that we want to follow is to try to convert our expressions to something similar to the hydrogenic partition function by means of averages of the energy and of sums of the statistical weights. The first sum of Equation (2) can be converted into

$$U_0 = \sum_{n=2}^{n'} \hat{g}_{nj} e^{-\frac{\hat{E}_{nj}}{k_B T}}, \quad (3)$$

where \hat{g}_{nj} is the sum of the statistical weights g_{nj} and \hat{E}_{nj} is the weighted average of the energies E_{nj} with respect to the statistical weights, for the shell n (Cowan 1981). Now applying the mean value theorem for sums to Equation (3), we can obtain the following expression:

$$\sum_{n=2}^{n'} \hat{g}_{nj} e^{-\frac{\hat{E}_{nj}}{k_B T}} = e^{-\frac{\bar{\xi}}{k_B T}} \sum_{n=2}^{n'} \hat{g}_{nj}, \quad (4)$$

where ξ is a value in the closed interval $(2, n')$, that is, $2 \leq \xi \leq n'$ as required by the theorem. Defining the sum in Equation (4) as

$$G_{jk} = \sum_{n=2}^{n'} \hat{g}_{nj} \hat{g}_{nk} \quad (5)$$

and taking ξ equal to the average energy with respect to the statistical weights \hat{g}_n gives

$$\xi = \mathcal{E}_{jk} = \frac{\sum_{n=2}^{n'} \hat{g}_{nj} \hat{g}_{nk} \hat{E}_{nj} \hat{E}_{nk}}{G_{jk}}, \quad (6)$$

that assures that ξ is in the interval $(2, n')$; therefore, Equation (3) becomes

$$U_0 = G_{jk} e^{-\frac{\mathcal{E}_{jk}}{k_B T}}. \quad (7)$$

The second sum of Equation (2) is defined as

$$U_1 = \sum_{n=n'}^{n^*} \hat{g}_{nj} \hat{g}_{nk} e^{-\frac{\hat{E}_{nj} \hat{E}_{nk}}{k_B T}}. \quad (8)$$

Using the results of Cardona et al. (2005), applying the mean value theorem for integrals, we obtain

$$U_1 = \frac{m}{3} (n^*{}^3 - n'^3) e^{-\frac{\hat{E}_{n^*jk}}{k_B T}}, \quad (9)$$

where m is the structure factor and comes from the quasi-hydrogenic approximation for the statistical weights $g_n = mn^2$ (Fischel & Sparks 1971), and defining the mean excitation energy of the last level in the atom as

$$\hat{E}_{n^*jk} = \chi_{jk} - \frac{Z_{\text{eff}}^2 Ry}{n^*{}^2}, \quad (10)$$

where χ_{jk} is the ionization potential of the ionization state j of the atomic species k considered, Ry is the energy of one Rydberg, and the effective charge $Z_{\text{eff}} = j + 1$, where j is the state of ionization of the ion, that is, $j = 0$ for neutral atoms and takes into account the screening of the core electrons in the atom. Now, the maximum level in the atom is given by (Cardona et al. 2005)

$$n^* = \frac{q}{2} \left(1 + \sqrt{1 + \frac{4}{q}} \right), \quad (11)$$

with

$$q = \sqrt{\frac{Z_{\text{eff}}}{2\pi a_0}} \frac{1}{\sqrt{N}}, \quad (12)$$

where a_0 is the Bohr radius and N is the total number of particles per unit volume of the material that composes the medium. Therefore, given the total number density N we can calculate n^* . The principal quantum number of the highest allowed state is given by other models also (Hummer & Mihalas 1988; Däppen et al. 1987). Substituting Equations (8) and (9) into Equation (2), we finally obtain

$$U = \hat{g}_{1jk} e^{-\frac{\hat{E}_{1jk}}{k_B T}} + G_{jk} e^{-\frac{\mathcal{E}_{jk}}{k_B T}} + \frac{m}{3} (n^*{}^3 - n'^3) e^{-\frac{\hat{E}_{n^*jk}}{k_B T}}. \quad (13)$$

This is our atomic partition function for any temperature and total number density with the four parameters G_{jk} , \mathcal{E}_{jk} , m , and n' . In order to comply with the requirements for the derivation

of Equation (9), using the mean value theorem for integrals, following the analysis of Cardona et al. (2009a), we set $n' = 7$. Therefore, Equation (13) gets transformed into the final form as

$$U = \hat{g}_{1jk} e^{-\frac{\hat{E}_{1jk}}{T}} + G_{jk} e^{-\frac{\mathcal{E}_{jk}}{T}} + \frac{m}{3} (n^*{}^3 - 343) e^{-\frac{\hat{E}_{n^*jk}}{T}}, \quad (14)$$

where the energies have been divided by the Boltzmann constant k_B . The parameters of the partition function are for each chemical element and each ionization stage of that element. Equation (14) is analytic; thus, the derivatives of Equation (14) with respect to N and T are given by

$$\left(\frac{dU}{dT} \right)_N = \hat{g}_{1jk} \frac{\hat{E}_{1jk}}{T^2} e^{-\frac{\hat{E}_{1jk}}{T}} + G_{jk} \frac{\mathcal{E}_{jk}}{T^2} e^{-\frac{\mathcal{E}_{jk}}{T}} + \frac{m}{3} \frac{\hat{E}_{n^*jk}}{T^2} (n^*{}^3 - 343) e^{-\frac{\hat{E}_{n^*jk}}{T}} \quad (15)$$

and

$$\left(\frac{dU}{dN} \right)_T = \frac{m}{3} \left[3n^*{}^2 \frac{dn^*}{dN} - \frac{(n^*{}^3 - 343)}{T} \frac{d\hat{E}_{n^*jk}}{dN} \right] e^{-\frac{\hat{E}_{n^*jk}}{T}}, \quad (16)$$

together with

$$\frac{d\hat{E}_{n^*jk}}{dN} = \frac{2Z_{\text{eff}}^2 Ry}{n^*{}^3} \frac{dn^*}{dN}, \quad (17)$$

$$\frac{dn^*}{dN} = \frac{1}{q} \left[n^* - \frac{1}{\sqrt{1 + \frac{4}{q}}} \right] \frac{dq}{dN}, \quad (18)$$

and

$$\frac{dq}{dN} = -\frac{1}{6} \frac{q}{N}. \quad (19)$$

Equation (14) together with Equations (15) and (16) are useful for any calculations of the equation of state in stellar atmospheres and interiors as well as for plasma diagnostics. This is the partition function that we will use to compare with other results in the following section.

3. RESULTS AND COMPARISONS

For model stellar atmospheres calculations, where the main thermodynamic variables are the temperature T and the total number density of particles N or the gas pressure P , our derived expressions are directly applicable. In order to make comparisons with other results it is necessary to calculate N for the given electron density n_e and to compile the required data from tables of the statistical weights and energy levels of the atoms, specially from the NIST physical data tables and from other sources. The statistical weights \hat{g}_{1jk} and the energies \hat{E}_{1jk} for the ground states of the atoms are given in tables as those of Cox (2000) and TOP (2009), or calculated from the tables of NIST (2009). In some cases, the energies \hat{E}_{1jk} are different from zero when the ground states are multiplets, but even so they are small. The procedure to obtain G_{jk} , \mathcal{E}_{jk} , and m is the following: the \hat{g}_{nj} for each shell n is obtained by adding up all the statistical weights collected from the tables of all the states in the shell, no matter if they are multiple excited. The energy \hat{E}_{nj} of the shell is obtained by making the weighted average of the energies E_{nj} with respect to the statistical weights for the shell

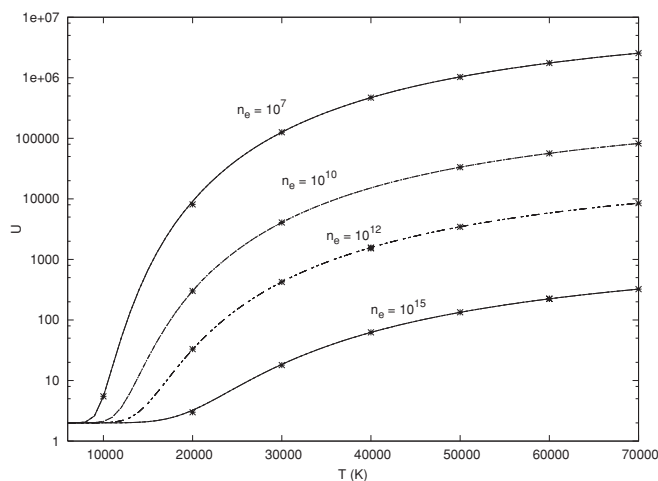


Figure 1. Curves of the partition function for hydrogen calculated with our results as a function of temperature for different electronic densities. The asterisks are the results of de Jager & Neven (1960) and from Fischel & Sparks (1971).

n , obtained from the tables. This procedure is carried out from $n = 2$ to $n = 7$. In this procedure, we try to simulate the hydrogenic calculations of the partition function. Now using Equations (5) and (6), we obtain G_{jk} and \mathcal{E}_{jk} . The structure parameters m is obtained by examining the list of total statistical weights of each shell n of the given atom using, $m = g_{njk}/n^2$ mentioned above, and one chooses the greater value among all the shells because it means that the shell has the greater number of levels. We have developed procedures and programs to retrieve the data from the tables of NIST and of TOP when necessary, of the energy levels of the atoms, to select the appropriate quantities up to the seventh shell in the atoms, in order to calculate the parameters of Equation (14). The procedures to retrieve the data and the necessary calculations to obtain the parameters for all the atomic species considered here are given in the following section. The comparisons of Equation (14) are made for three chemical species: hydrogen, helium, and nitrogen, because there are published results of the partition function of these elements and their ions.

For hydrogen there are several comparison that one can make. The first one is carried out using the combination of Equations (3) and (9), setting $n' = 7$ in order to compare with our partition function. This would test the accuracy of the second term of Equation (14). The second one is the comparison of the combination of Equations (3) and (9) with the evaluation of the original partition function with the upper limit set equal to n^* . The third one is the comparison of our result with the direct calculation of the partition function using

$$E_n = \chi_{01} - \frac{Ry}{n^2}, \quad (20)$$

that is similar to Equation (10), where χ_{01} is the ionization potential of neutral hydrogen and $g_n = 2n^2$ in Equation (1) with the upper limit set equal to n^* . The calculations are carried out for some electron densities n_e and temperatures T using the standard procedures (Mihalas 1978; Cardona et al. 2009b) to obtain the total number density of particles N necessary in the calculation of n^* . Figure 1 shows the curves for the values of the partition function calculated using the three forms of the partition function mentioned above for several electron densities, 10^7 , 10^{10} , 10^{12} , and 10^{15} cm^{-3} , as a function of temperature. The results behave in a similar way with respect

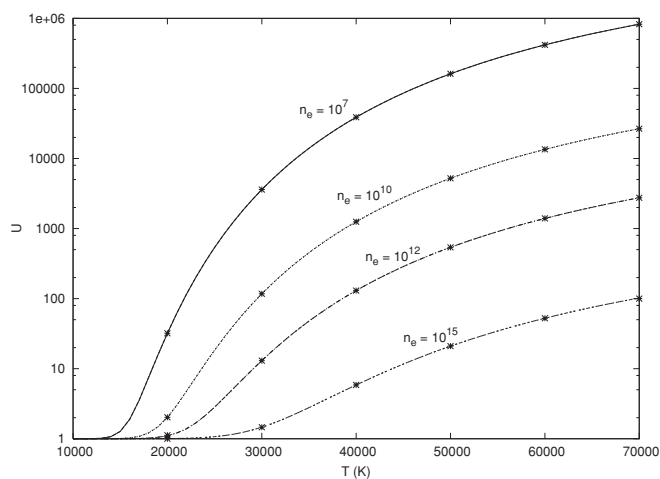


Figure 2. Curves of the partition function for neutral helium calculated with our results as a function of temperature for different electronic densities. The asterisks are the results of de Jager & Neven (1960) and from Fischel & Sparks (1971).

to the exact evaluation of the partition function for hydrogen. The relative errors are less than 0.1% for all temperature and for electron densities less than 10^{15} cm^{-3} . Therefore, the results of the three different evaluations of the partition function are not appreciated in the scale of the figures. The interpolated results of de Jager & Neven (1960) and of Fischel & Sparks (1971) for the electron densities considered have higher relative errors with respect to the direct evaluation of the partition function. For low temperatures and high densities, there are few levels in the atoms; for example, for temperatures around 10^4 K and electron densities of around 10^{16} cm^{-3} , the number of levels that remain in the atoms, given by Equation (11), is of the order of 5 that agree with the experimental values for the Balmer lines of hydrogen where only three lines appear, as can be seen in Figure 1.7 of Fujimoto (2005) and Figures 5.5 of Griem (1997). Therefore, our expression would fail under these conditions and one has to calculate Equation (1) directly for the few levels given. Then, Equation (14) is a good representation of Equation (1), when there are a sufficient number of terms in the atoms, let say more than 12. When there are seven levels in the atoms one uses only the two first terms of Equation (14). The evaluation of the partition function for hydrogen is important because we have the possibility of directly compare with the exact evaluation of the partition function, something that we cannot do with the other elements, except the hydrogenic ones.

For helium we can compare with the interpolated results of de Jager & Neven (1960) and Fischel & Sparks (1971). The results of the calculations for He I are shown in Figure 2 for the same electronic densities given above. The relative errors for the temperatures shown are of the order of few percent; thus, the results from Equations (3) and (9) are not seen in the scale of the figure. For He II, Figure 3 shows the curves for the derived partition function for the electronic densities given above with respect to temperature, the relative errors with respect to the direct evaluation of the partition function, as for hydrogen, are less than 0.5% and with respect to the interpolated results of Fischel & Sparks (1971) are of the order of a few percent also. The results of de Jager & Neven (1960) are very far away from our results and of the results of Fischel & Sparks (1971). We do not know the reasons for that difference.

For nitrogen, we present results for N I, N II, and N III, since there are results reported in the literature for them. The

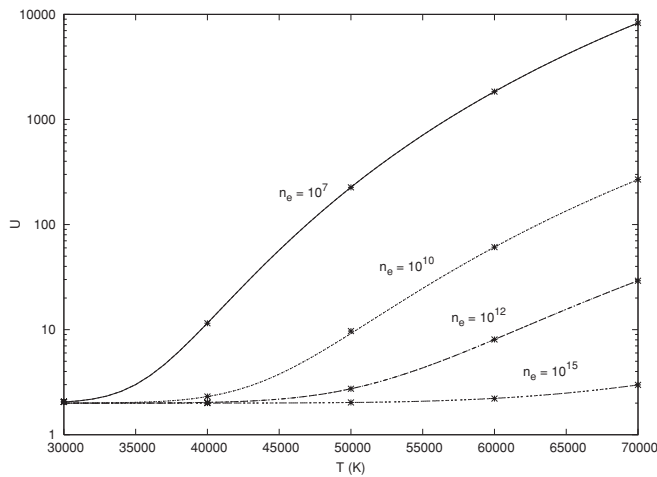


Figure 3. Curves of the partition function for ionized Helium calculated with our results as a function of temperature for different electronic densities. The asterisks are the results of Fischel & Sparks (1971).

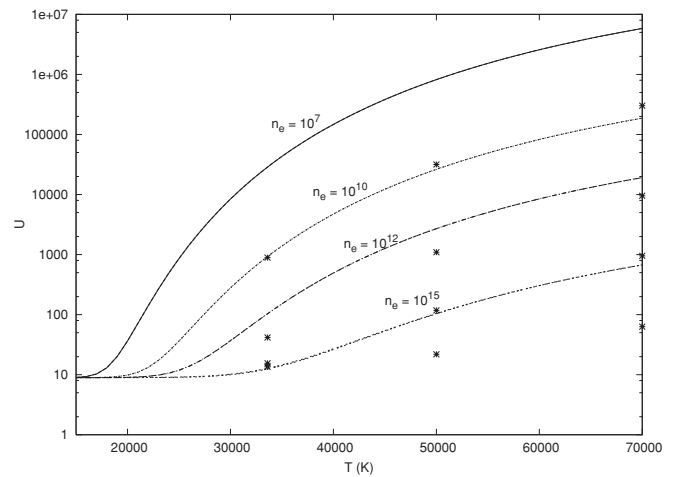


Figure 5. Curves of the partition function for ionized Nitrogen calculated with our results as a function of temperature for different electronic densities. The asterisks are the results of de Jager & Neven (1960).

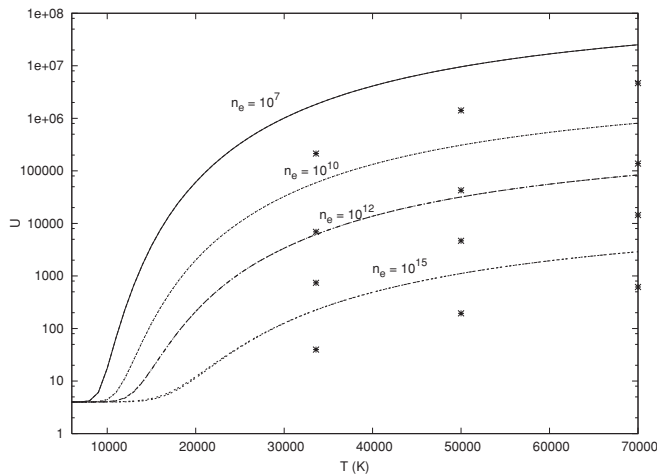


Figure 4. Curves of the partition function for neutral Nitrogen calculated with our results as a function of temperature for different electronic densities. The asterisks are the results from de Jager & Neven (1960).

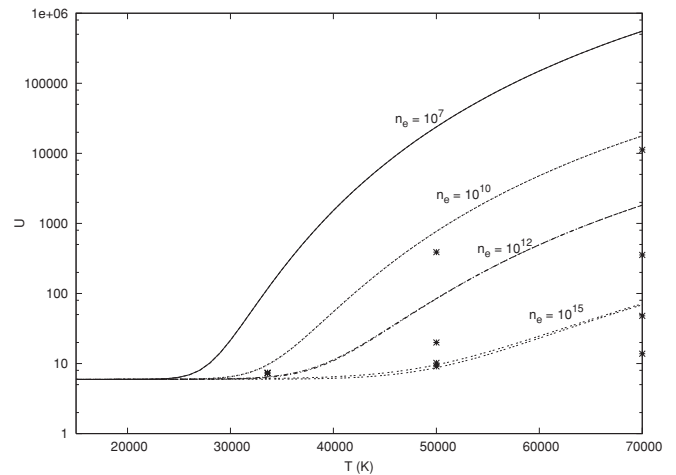


Figure 6. Curves of the partition function for double ionized Nitrogen calculated with our results as a function of temperature for different electronic densities. The asterisks are the results of de Jager & Neven (1960).

comparisons are carried out using our partition function and the combination of Equations (3) and (9), as was done for hydrogen and helium, with the derived results of de Jager & Neven (1960). Figure 4 shows the calculations for N I, Figure 5 the calculations for N II, and Figure 6 the calculated values for N III, all of them for the electronic densities given above. The results for the ions of nitrogen do not compare at all with calculated points of de Jager & Neven (1960); the asterisks are farther down than their respective curves in the figures, one cannot determine the cause of the differences, and Fischel & Sparks (1971) conclude that the use of an incorrect value of the structure factor m produces wrong results for N I, and an insufficient number of terms for N II is the cause of the differences. For N III, our results do not compare with the values reported by de Jager & Neven (1960) shown by the asterisks. For high densities, our results are different from the results of the combination of Equations (3) and (9) due to the low number of level at those densities. Another cause for the differences is that de Jager & Neven (1960) did not take into account the double excited energy states in nitrogen. Therefore, other comparison that one can make is to consider the case of atoms with and without the double excited state, and for that purpose we use N II with and without the double excited

states and the results are shown in Figure 7 where the upper curves for each electronic density are the ones with the double excited states taken into account. Those results could not explain the differences with the results of de Jager & Neven (1960). Also, we cannot compare our results with other computations such as the ones of Irwin (1981) and Sauval & Tatum (1984) because the partition function is calculated truncating the sum of the partition function to a particular excitation energy and not necessarily to the correct result given, for example, by Equation (11) or by other sources (Hummer & Mihalas 1988), and also the range in temperatures considered is very small.

We cannot compare the derivatives of the partition function obtained above with other derivations because we do not have any information about other results. Nevertheless, we can compare with the exact derivatives of the partition function with respect to temperature and total number density of particles for the hydrogenic ions. For the derivative with respect to temperature, we can use the definition of the partition function with the upper limit set to the maximum level n^* , giving relative errors of less than 1% for the conditions mentioned above. For the derivative with respect to the total number density of particles N , we can compare with the exact derivative for the hydrogenic

Table 1
Free Parameters of the Partition Function

Z	J	\mathcal{E}	G	m	Z	J	\mathcal{E}	G	m	Z	J	\mathcal{E}	G	m
1	0	150991.49	278	2	12	4	1411093.36	647	21*	17	4	**		
2	0	278302.52	556	4	12	5	1865964.26	1418	31*	17	5	**		
2	1	604233.37	278	2	12	6	2142223.03	1010	31*	17	6	1007399.32	236	2
3	0	52534.09	124	2	12	7	2338880.38	576	29*	17	7	3539215.89	99	2
3	1	839918.28	299	4	12	8	2773140.05	318	14	17	8	**		
3	2	1359687.21	278	2	12	9	3261657.47	120	2	17	9	**		
4	0	96994.39	318	7	12	10	19189623.12	266	4	17	10	**		
4	1	183127.29	250	2	12	11	21237123.02	124	2	17	11	**		
4	2	1687543.18	234	4	13	0	61332.91	226	2	17	12	**		
4	3	2417471.50	278	2	13	1	186963.72	456	9	17	13	**		
5	0	82608.14	152	6	13	2	270429.14	242	2	17	14	**		
5	1	254450.62	427	15	13	3	1216959.19	545	12	17	15	**		
5	2	361450.28	166	2*	13	4	1549146.53	1170	31*	17	16	**		
5	3	2843419.75	260	4*	13	5	1886238.18	1083	28*	18	0	175362.78	1156	12
5	4	3777763.90	278	2	13	6	2414611.81	1204	21*	18	1	291708.85	2642	29
6	0	119011.30	755	12	13	7	2812666.21	1755	33*	18	2	332987.89	654	22*
6	1	247141.75	412	15	13	8	2542105.04	334	21*	18	3	537020.33	1276	23*
6	2	481799.03	619	16	13	9	3548579.89	373	12*	18	4	676953.56	780	11*
6	3	638971.96	262	2	13	10	3916731.05	120	2	18	5	689723.48	386	16*
6	4	4372895.09	526	4	13	11	22713375.11	266	4	18	6	899714.78	278	11
6	5	5440754.24	278	2	13	12	24893674.25	120	2	18	7	1226291.38	216	2
7	0	156577.63	1076	23	14	0	84557.15	810	12	18	8	4276148.89	758	12*
7	1	297149.04	826	23	14	1	159923.67	354	15	18	9	4765524.26	1810	31*
7	2	463576.22	532	22	14	2	327359.79	685	12	18	10	5427874.79	2126	69*
7	3	761375.52	637	16	14	3	424109.62	268	2	18	11	6309262.74	1942	35*
7	4	969809.93	276	2	14	4	1734718.76	816	12*	18	12	6891291.49	3442	92*
7	5	5955082.97	161	4	14	5	2052871.62	898	30*	18	13	6930433.44	1968	56*
7	6	7406739.18	278	2	14	6	2366175.20	527	17*	18	14	7939677.47	947	16*
8	0	148025.55	658	10	14	7	3068684.69	1804	27*	18	15	8000300.84	96	2*
8	1	358811.61	1104	33	14	8	3544292.35	2157	36*	18	16	44488328.97	179	4*
8	2	522198.02	769	39	14	9	2939472.35	274	17*	18	17	49025928.61	278	2*
8	3	770292.81	812	37	14	10	4284733.99	440	12*	19	0	41649.47	154	2
8	4	1127189.72	805	16	14	11	4631575.50	120	2	19	1	**		
8	5	1337937.59	228	2	14	12	26837561.59	376	4	19	2	**		
8	6	8063119.12	230	4	14	13	28926125.27	124	2	19	3	**		
8	7	9676005.18	278	2	15	0	111553.41	1438	21	19	4	**		
9	0	189306.98	642	22	15	1	187200.91	673	13	19	5	**		
9	1	369967.32	1072	33	15	2	279091.88	524	20	19	6	**		
9	2	648202.69	2070	43*	15	3	490515.56	782	16	19	7	1123307.05	320	10
9	3	862099.86	1285	45*	15	4	599981.58	268	2	19	8	1408338.41	144	2
9	4	1081435.70	674	36*	15	5	2035495.04	248	12	19	9	**		
9	5	1410884.98	381	14	15	6	**			19	10	**		
9	6	1777557.76	198	2	15	7	**			19	11	**		
9	7	10507621.11	308	4	15	8	**			19	12	**		
9	8	12248930.42	278	2	15	9	**			19	13	**		
10	0	242506.72	1200	12	15	10	**			19	14	**		
10	1	445257.78	2030	29	15	11	**			19	15	**		
10	2	657825.06	1391	40	15	12	**			19	16	**		
10	3	948042.58	908	26*	15	13	31007596.77	376	4	19	17	**		
10	4	1229305.92	1373	40*	15	14	33218858.77	124	2	19	18	**		
10	5	1402396.67	614	41	16	0	109679.73	660	13	20	0	59040.50	414	10
10	6	1984373.15	758	16	16	1	226987.56	1388	29	20	1	104428.91	184	2
10	7	2249518.89	174	2	16	2	295403.69	463	12*	20	2	510019.07	931	12
10	8	13035747.69	237	4	16	3	418347.48	648	22	20	3	558657.22	620	22*
10	9	15125862.09	278	2	16	4	646590.95	616	12	20	4	708820.36	329	8*
11	0	53037.84	268	2	16	5	793008.25	250	2	20	5	1016510.46	1614	26*
11	1	514746.96	836	12	16	6	2548457.94	242	12	20	6	1163436.41	1083	16*
11	2	748590.86	1156	30*	16	7	3335040.66	1284	24*	20	7	895168.86	174	8
11	3	967135.82	841	37*	16	8	3808539.43	1065	26*	20	8	1331538.08	321	10
11	4	1399246.48	1316	31*	16	9	4539809.54	1946	35*	20	9	1675252.51	144	2
11	5	1663176.34	1052	33*	16	10	5061921.17	2109	36*	20	10	6264642.54	873	10*
11	6	1880070.95	628	34	16	11	3920308.38	246	14	20	11	6675525.78	2104	48*
11	7	2420828.30	421	13*	16	12	5836111.97	366	9*	20	12	7300369.62	2724	86*
11	8	2627246.17	106	2	16	13	6237904.34	118	2*	20	13	8271825.80	3730	103*
11	9	15982554.64	260	4	16	14	35480563.25	376	4	20	14	9069080.36	4227	112*
11	10	17839645.56	124	2	16	15	38723116.45	278	2*	20	15	9213595.25	794	22*

Table 1
(Continued)

Z	J	\mathcal{E}	G	m	Z	J	\mathcal{E}	G	m	Z	J	\mathcal{E}	G	m
12	0	80322.99	421	5	17	0	141057.47	1344	21	20	16	10293633.64	849	16*
12	1	148041.70	252	2	17	1	239116.84	1444	34	20	17	10010271.91	102	2
12	2	828015.89	531	12	17	2	**			20	18	55504272.68	136	4*
12	3	1134464.90	1536	31*	17	3	**			20	19	60549406.08	278	2*

Notes. “**” indicates data taken from the NIST and TOP databases. “***” indicates sufficient information not available.

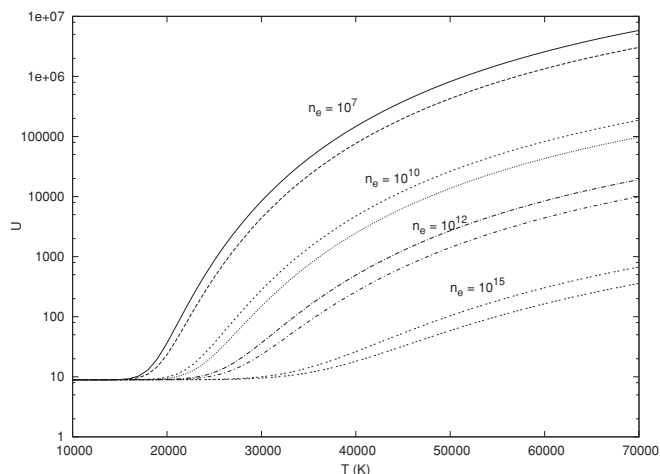


Figure 7. Curves of the partition function for ionized nitrogen calculated with and without the double excited states as a function of temperature for different electronic densities. The lower curves for each series are for N II without the double excited states.

atom given by

$$\left(\frac{dU}{dN}\right)_T = mn_*^2 e^{-\frac{\hat{E}_{n*jk}}{T}} \frac{dn_*}{dN}, \quad (21)$$

producing relative error of less than 1% for the same conditions. All of these comparisons validate the derivation of our partition function.

4. TABLE OF PARAMETERS

The procedures for selecting and retrieving the data from the tables are presented in this section. We decided to use the data bases of NIST and TOP because they are the most complete set of atomic data. The data base of NIST contains the atomic configurations, the energy levels in cm^{-1} and the total angular momentum of the chemical elements and some other spectroscopy information. For our purpose, we use the tables of energy levels of the atoms and their ions. When necessary we use the TOP data base that gives the atomic configurations, the energy levels in Rydberg, and the statistical weights directly. The two data bases complement each other in different ways. Some times there are atomic ions in one data base that have incomplete energy levels necessary for our purposes and then we use the one that has more information. Also, there exist levels in one ion that do not have the same energy in the two systems, especially of the double excited energy states, for example in single ionized beryllium. In some cases, we use a combination of both data bases.

We have compiled the data from the ground states up to the seventh shells. The seventh shell was chosen due to theoretical

and mathematical reasons. For instance, in the derivation of the third term of our partition function, in order to produce an analytic function, it is required to transform the sum into an integral. Therefore, it is necessary that the levels should be close enough to each other, practically forming a continuum; thus, from the arguments of Cardona et al. (2009a), this is accomplished setting the maximum shell n equal to 7. There exist ions in the two data set that do not have levels up to the seventh shell and as we do not have any other information, that ion is not taken into account in our table. The multiple excited states with different parent ions are taken into account in the averaging as, if they were in the same shell, together with the single excited states. The procedures and programs to retrieve the data from the data bases are available upon request.

Table 1 contains the values of the free parameters of the partition function given in Equation (14). Column 1 represents the atomic number, Z , Column 2 the ionization stage, J , Column 3 the excitation energies, \mathcal{E}_{jk} , Column 4 the statistical weights, G_{jk} , and Column 5 represents the structure factors, m . These columns are repeated twice. The remaining quantities $\hat{g}_{1,jk}$ and $\hat{E}_{1,jk}$ of the ground states are obtained from the tables mentioned before, and n_* and \hat{E}_{n*jk} are calculated from the formulas given above, using the given temperatures and total number densities of particles with the ionization potentials given in the tables mentioned before. The data required to obtain the free parameters of the partition function in Table 1 are available upon request.

5. CONCLUSIONS AND COMMENTARIES

We have derived the atomic partition function for applications in stellar atmospheres and plasma diagnostics supposing that one can simulate the calculations of the partition function for atomic hydrogen where the levels in a given shell have the same energy; they are degenerate in energy. For that purpose, we have used the mean value theorems for integrals and sum to obtain mean values for the energies and statistical weights and an analytic function in terms of these mean values and a structure factor. The comparisons with some published values of the partition function in the literature are in accordance with the results of our derived partition function. The tables of the free parameters provided can be used for the calculation of the partition function for the given elements for any temperature and total number density of particles in the particular system under study. This partition function can be used in the calculation of the equation of state following the procedures of Cardona et al. (2009b) and the procedures that use the Helmholtz free-energy minimization methods (Mihalas et al. 1988).

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