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PARTITION FUNCTION OF B I AND B II

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Abstract: Recent measurements of energy levels in B I and B II enabled us to calculate their partition functions. The results are tabulated in a temperature interval from 5000 to 35 000 K.

1. Introduction

The partition functions of B I and B II are absent from the tables of Drawin and Felenbok[1]. However, recently published papers[2-5] together with earlier ones[6-9] supply sufficient data for the computation of these partition functions.

Partition function is defined as a sum

$$Z(T) = \sum_{n=1}^{n^*} g_n \exp\left(-\frac{E_n}{kT}\right), \tag{1}$$

where g_n and E_n are the statistical weight and energy of the n-th level, respectively, n^* is the last level in the atom, lying just below the ionization limit, k the Boltzmann constant and T the temperature of the plasma. Regarded as an isolated system the atom possesses an infinite number of states which causes a divergence of the par-

tition function. However due to mutual interaction with the surrounding plasma the ionization potential of the atom decreases, leaving it with a finite number of states. For a practical computation of the partition function it is useful to have a minimum number of terms in Equ. (1). This can be successfully achieved by approximating higher energy levels by hydrogenic levels. Summation over hydrogenic levels may be replaced by an integral resulting in the following expression for the partition function[10]

$$Z(T) = \sum_{n=1}^{n'} g_n \exp\left(-\frac{E_n}{kT}\right) + \frac{3}{2}(2S_1 + 1)(2L_1 + 1)\left(\frac{E_H}{E_\infty}\right)^{\frac{3}{2}} \exp - \left(\frac{E_\infty}{kT} - \right.$$
$$\left. - \frac{\Delta E_\infty}{kT}\right), \tag{2}$$

where S_1 and L_1 are the total spin and orbital angular momentum of the parent ion. E_H is the ionization energy of hydrogen, E_∞ the ionization energy of the isolated atom, ΔE_∞ the lowering of the ionization energy, and n' the last principal quantum number for which all sublevels are experimentally determined. For experimental purposes in plasma spectroscopy it is sufficient to take into account only the sum on the right side of the equation (2).

In complex atoms, even at relatively low temperatures, several different configurations of electrons may be realized. Each configuration may be regarded as a separate atom with its own energy levels and ionization potential. In order to apply the approximate formula (2) to such a complex system, summation over all configurations have to be performed resulting in the following relation

$$Z(T) = \sum_{i=1}^{N} \sum_{n=1}^{n'(i)} g_n^{(i)} \exp\left(-\frac{E_n^{(i)}}{kT}\right) + \sum_{n=1}^{N} \frac{3}{2}(2S_1^{(i)} + 1)(2L_1^{(i)} +$$
$$+ 1)\left(\frac{E_H}{E_\infty}\right)^{\frac{3}{2}} \exp\left(-\frac{(E_\infty^{(i)} - \Delta E_\infty^{(i)})}{kT}\right), \tag{3}$$

where the summation over the index (i) is carried out over all the configurations. However, in practical calculations summation over configurations is reduced to only a few terms. If the excitation of the parent ion does not disturb the hydrogenic part of the atomic potential, then ΔE_∞ is the same for such different configurations*. Generally, only the levels which converge towards the first ionization potential are well known, and only, a few levels of other configurations. Thus, the contribution of the different configurations to the partition function may be

*H. W. Darwin, private communication.

assessed by a comparison of their hydrogenic parts. As an example of such comparison we give B I, the first ionization potential of which is 8.3 eV and the second about 11.3 eV. At a temperature of 20 000 K, where B I is almost completely ionized, the contribution of the hydrogenic part of the second configuration is less than 20% of the hydrogenic contribution of the first configuration.

2. *Procedure*

In our calculations, the hydrogenic level approximation was taken into account only for the levels which converge towards the first ionization limit. All levels from other configurations, which are known from experiment, have been taken into account in the calculations.

We used the same tabulation method as that by Drawin and Felenbok[1] i. e. the values of the partitition function are tabulated as a function of temperature and of the lowering ionization potential. In the case of B I summation over discrete levels have been performed up to the nineth principal quantum number. For the energy of the levels which have not been experimentally observed we used the approximate values predicted by the Ritz formula and, for the energies of the G, H, I, J, and K levels, hydrogenic values. For B II, which is a beryllium-like ion, summation was carried out up to the principal quantum number six.

Acknowledgement

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PARTITION FUNCTION VALUES OF B I

T K \ ΔE eV	.05	.10	.25	.50	1.00	2.00	3.00
5000	5.98468	5.98468	5.98468	5.98467	5.98467	5.98467	5.98467
5200	5.98757	5.98757	5.98756	5.98756	5.98755	5.98755	5.98754
5600	5.99109	5.99109	5.99108	5.99106	5.99105	5.99104	5.99102
5900	5.99543	5.99543	5.99540	5.99537	5.99535	5.99533	5.99528
6200	6.00078	6.00078	6.00071	6.00066	6.00061	6.00056	6.00049
6500	6.00734	6.00734	6.00720	6.00709	6.00699	6.00691	6.00678
6800	6.01532	6.01532	6.01504	6.01484	6.01466	6.01452	6.01432
7100	6.02493	6.02493	6.02444	6.02407	6.02377	6.02354	6.02322
6400	6.03641	6.03641	6.03557	6.03494	6.03445	6.03409	6.03362
7700	6.05002	6.05002	6.04864	6.04762	6.04684	6.04629	6.04561
8000	6.06604	6.06604	6.06386	6.06226	6.06105	6.06024	6.05928
8300	6.08476	6.08476	6.08142	6.07899	6.07720	6.07603	6.07472
8600	6.10652	6.10652	6.10156	6.09798	6.09537	6.09374	6.09198
8900	6.13167	6.13167	6.12450	6.11935	6.11567	6.11344	6.11113
9200	6.16061	6.16061	6.15048	6.14325	6.13817	6.13518	6.13219
9500	6.19373	6.19373	6.17974	6.16982	6.16293	6.15900	6.15520
9800	6.23149	6.23149	6.21255	6.19917	6.19003	6.18494	6.18017
10100	6.27434	6.27434	6.24916	6.23145	6.21950	6.21302	6.20713
10400	6.32279	6.32279	6.28983	6.26678	6.25140	6.24326	6.23606
10700	6.37732	6.37732	6.33486	6.30527	6.28576	6.27566	6.26697
11000	6.43847	6.43847	6.38450	6.34705	6.32261	6.31023	6.29984
11300	6.50677	6.50677	6.43904	6.39223	6.36197	6.34696	6.33466
11600	6.58276	6.58276	6.49875	6.44090	6.40387	6.38585	6.37141
11900	6.66698	6.66698	6.56391	6.49318	6.44831	6.42687	6.41006
12200	6.75998	6.75998	6.63478	6.54916	6.49530	6.47001	6.45059
12500	6.86229	6.86229	6.71163	6.60893	6.54485	6.51524	6.49296
12800	6.97444	6.97444	6.79472	6.67258	6.59694	6.56255	6.53714
13100	7.09696	7.09696	6.88429	6.74016	6.65157	6.61189	6.58309
13400	7.23035	7.23035	6.98057	6.81177	6.70873	6.66324	6.63078
13700	7.37510	7.37510	7.08380	6.88746	6.76841	6.71656	6.68018
14000	7.53167	7.53167	7.19419	6.96728	6.83059	6.77182	6.73123
14300	7.70051	7.70051	7.31192	7.05129	6.89523	6.82899	6.78391
14600	7.88204	7.88204	7,43720	7.13953	6.96233	6.88801	6.83817
14900	8.07666	8.07666	7.57019	7.23202	7.03185	6.94886	6.89398
15200	8.28474	8.28474	7.71105	7.32880	7.10377	7.01149	6.95128
15500	8.50663	8.50663	7.85991	7.42989	7.17804	7.07587	7.01005
15800	8.74264	8.74264	8.01691	7.53530	7.25464	7.14195	7.07024
16100	8.99305	8.99305	8.18215	7.64504	7.33354	7.20968	7.13181
16400	9.25813	9.25813	8.35573	7.75910	7.41468	7.27904	7.19472
16700	9.53810	9.53810	8.53774	7.87749	7.49805	7.34997	7.25894
17000	9.83317	9.83317	8.72823	8.00019	7.58358	7.42244	7.32442
17300	10.14351	10.14351	8.92726	8.12719	7.67126	7.49640	7.39113
17600	10.46926	10.46926	9.13487	8.25846	7.76102	7.57181	7.45903
17900	10.81056	10.81056	9.35108	8.39398	7.85283	7.64863	7.52809
18200	11.16748	11.16748	9.57590	8.53371	7.94665	7.72682	7.59826
18500	11.54010	11.54010	9.80933	8.67762	8.04243	7.80635	7.66952
18800	11.92847	11.92847	10.05137	8.82566	8.14012	7.88716	7.74182
19100	12.33260	12.33260	10.30198	8.97780	8.23969	7.96922	7.81513
19400	12.75249	12.75249	10.56114	9.13398	8.34108	8.05249	7.88943
19700	13.18812	13.18812	10.82879	9.29416	8.44425	8.13694	7.96467
20000	13.63945	13.63945	11.10488	9.45827	8.54915	8.22252	8.04083
20300	14.10641	14.10641	11.38935	9.62627	8.65574	8.30920	8.11787
20600	14.58892	14.58892	11.68212	9.79809	8.76398	8.39694	8.19577

PARTITION FUNCTION VALUES OF B I [Continued]

ΔE eV / T K	.05	.10	.25	.50	1.00	2.00	3.00
20900	15.08690	15.08690	11.98312	9.97366	8.87381	8.48570	8.27449
21200	15.60021	14.60021	12.29227	10.15293	8.98520	8.57546	8.35400
21500	16.12874	16.12874	12.60945	10.33583	9.09809	8.66617	8.43427
21800	16.67233	16.67233	12.93458	10.52228	9.21244	8.75780	8.51528
22100	17.23084	17.23084	13.26755	10.71223	9.32821	8.85032	8.59701
22400	17.80410	17.80410	13.60824	10.90560	9.44535	8.94369	8.67941
22700	18.39192	18.39192	13.95655	11.10231	9.56383	9.03788	8.76247
23000	18.99412	18.99412	14.31234	11.30230	9.68359	9.13287	8.84616
23300	19.61051	19.61051	14.67550	11.50549	9.80459	9.22861	8.93046
23600	20.24086	20.24086	15.04590	11.71181	9.92680	9.32508	9.01533
23900	20.88497	20.88497	15.42340	11.92119	10.05017	9.42226	9.10076
24200	21.54261	21.54261	15.80788	12.13354	10.17466	9.52010	9.18673
24500	22.21356	22.21356	16.19920	12.34879	10.30023	9.61859	9.27321
24800	22.89759	22.89759	16.59721	12.56688	10.42684	9.71769	9.36018
25100	23.59445	23.59445	17.00178	12.78772	10.55445	9.81738	9.44761
25400	24.30390	24.30390	17.41277	13.01123	10.68302	9.91763	9.53549
25700	25.02570	25.02570	17.83004	13.23735	10.81252	10.01842	9.62379
26000	25.75959	25.75959	18.25344	13.46601	10.94290	10.11972	9.71250
26300	26.50533	26.50533	18.68283	13.69712	11.07414	10.22150	9.80159
26600	27.26267	27.26267	19.11807	13.93061	11.20620	10.32374	9.89105
26900	28.03134	28.03134	19.55901	14.16642	11.33903	10.42643	9.98086
27200	28.81108	28.81108	20.00550	14.40447	11.47262	10.52953	10.07099
27500	29.60165	29.60165	20.45742	14.64468	11.60691	10.63302	10.16144
27800	30.40279	30.40279	20.91460	14.88700	11.74189	11.73688	10.25218
28100	31.21423	31.21423	21.37691	15.13134	11.87752	10.84109	10.34320
28400	32.03573	31.03573	21.84421	15.37764	12.01376	10.94563	10.43447
28700	32.86702	32.86702	22.31636	15.62584	12.15059	11.05049	10.52599
29000	33.70785	33.70785	22.79322	15.87586	12.28797	11.15563	10.61774
29300	34.55797	34.55797	23.27465	16.12765	12.42588	11.26104	10.70971
29600	35.41713	35.41713	23.76051	16.38112	12.56429	11.36670	10.80187
29900	36.28506	36.28506	24.25066	16.63623	12.70317	11.47260	10.89421
30200	37.16154	37.16154	24.74498	16.89291	12.84250	11.57871	10.98673
30500	38.04630	38.04630	25.24333	17.15109	12.98223	11.68502	11.07940
30800	38.93910	38.93910	25.74558	17.41072	13.12236	11.79151	11.17221
31100	39.83972	39.83972	26.25159	17.67174	13.26285	11.89817	11.26515
31400	40.74789	40.74789	26.76125	17.93408	13.40368	12.00498	11.35821
31700	41.66340	41.66340	27.27442	18.19770	13.54482	12.11192	11.45137
32000	42.58600	42.58600	27.79099	18.46252	13.68626	12.21898	11.54463
32300	43.51546	43.51546	28.31082	18.72851	13.82796	12.32614	11.63796
32600	44.45157	44.45157	28.83381	18.99560	13.96991	12.43340	11.73137
32900	45.39409	45.39409	29.35982	19.26374	14.11209	12.54073	11.82483
33200	46.34281	46.34281	29.88875	19.53288	14.25446	12.64813	11.91834
33500	47.29750	47.29750	30.42048	19.80297	14.39702	12.75557	12.01188
33800	48.25796	48.25796	30.95490	20.07395	14.53974	12.86305	12.10545
34100	49.22396	49.22396	31.49190	20.34579	14.68260	12.97056	12.19904
34400	50.19532	50.19532	32.03137	20.61842	14.82559	13.07808	12.29264
34700	51.17182	51.17182	32.57320	20.89181	14.96867	13.18560	12.38623
35000	52.15325	52.15325	33.11729	21.16591	15.11185	13.29311	12.47981

PARTITION FUNCTION VALUES OF B II

T K \ ΔE eV	.05	.10	.25	.50	1.00	2.00	3.00
5000	1.00019	1.00019	1.00019	1.00019	1.00019	1.00019	1.00019
5300	1.00036	1.00036	1.00036	1.00036	1.00036	1.00036	1.00036
5600	1.00061	1.00061	1.00061	1.00061	1.00061	1.00061	1.00061
5900	1.00100	1.00100	1.00100	1.00100	1.00100	1.00100	1.00100
6200	1.00155	1.00155	1.00155	1.00155	1.00155	1.00155	1.00155
6500	1.00231	1.00231	1.00231	1.00231	1.00231	1.00231	1.00231
6800	1.00333	1.00333	1.00333	1.00333	1.00333	1.00333	1.00333
7100	1.00465	1.00465	1.00465	1.00465	1.00465	1.00465	1.00465
7400	1.00632	1.00632	1.00632	1.00632	1.00632	1.00632	1.00632
7700	1.00838	1.00838	1.00838	1.00838	1.00838	1.00838	1.00838
8000	1.01089	1.01089	1.01089	1.01089	1.01089	1.01089	1.01089
8300	1.01389	1.01389	1.01389	1.01389	1.01389	1.01389	1.01389
8600	1.01741	1.01741	1.01741	1.01741	1.01741	1.01741	1.01741
8900	1.02149	1.02149	1.02149	1.02149	1.02149	1.02149	1.03149
9200	1.02618	1.02618	1.02618	1.02618	1.02618	1.02618	1.02618
9500	1.03149	1.03149	1.03149	1.03149	1.03149	1.03149	1.03149
9800	1.03745	1.03745	1.03745	1.03745	1.03745	1.03745	1.03745
10100	1.04410	1.04410	1.04410	1.04410	1.04410	1.04410	1.04410
10400	1.05143	1.05143	1.05143	1.05143	1.05143	1.05143	1.05143
10700	1.05947	1.05947	1.05947	1.05947	1.05947	1.05947	1.05947
11000	1.06823	1.06823	1.06823	1.06823	1.06823	1.06823	1.06823
11300	1.07772	1.07772	1.07772	1.07772	1.07772	1.07772	1.07772
11600	1.08794	1.08794	1.08794	1.08794	1.08794	1.08794	1.08794
11900	1.09890	1.09890	1.09890	1.09890	1.09890	1.09890	1.09890
12200	1.11059	1.11058	1.11058	1.11058	1.11058	1.11058	1.11058
12500	1.12300	1.12300	1.12300	1.12300	1.12300	1.12300	1.12300
12800	1.13615	1.13615	1.13614	1.13614	1.13614	1.13614	1.13614
13100	1.15001	1.15001	1.15000	1.15000	1.15000	1.15000	1.15000
13400	1.16459	1.16458	1.16458	1.16457	1.16457	1.16457	1.16457
13700	1.17987	1.17986	1.17985	1.17985	1.17985	1.17984	1.17984
14000	1.19585	1.19582	1.19581	1.19581	1.19581	1.19581	1.19581
14300	1.21252	1.21247	1.21245	1.21245	1.11245	1.21245	1.21245
14600	1.22986	1.22979	1.22976	1.22976	1.22976	1.22975	1.22975
14900	1.24787	1.24777	1.24773	1.24772	1.24772	1.24771	1.24771
15200	1.26655	1.26640	1.26634	1.26632	1.26632	1.26631	1.26631
15500	1.28588	1.28566	1.28558	1.28556	1.28555	1.28554	1.28553
15800	1.30586	1.30556	1.30543	1.30540	1.30539	1.30538	1.30537
16100	1.32650	1.32607	1.32589	1.32585	1.32584	1.32581	1.32581
16400	1.34779	1.34719	1.34694	1.34689	1.34687	1.34684	1.34683
16700	1.36975	1.36892	1.36858	1.36850	1.36847	1.36843	1.36842
17000	1.39237	1.39125	1.39078	1.39068	1.39064	1.39059	1.39057
17300	1.41569	1.41418	1.41355	1.41341	1.41336	1.41329	1.41327
17600	1.43972	1.43770	1.43687	1.43668	1.43661	1.43652	1.43649
17900	1.46449	1.46183	1.46073	1.46048	1.46039	1.46027	1.46023
18200	1.49004	1.48657	1.48513	1.48480	1.48468	1.48453	1.48448
18500	1.51643	1.51193	1.51006	1.50964	1.50949	1.50929	1.50923
18800	1.54371	1.53792	1.53552	1.53498	1.53478	1.53453	1.53446
19100	1.57195	1.56457	1.56151	1.56082	1.56057	1.56025	1.56016
19400	1.60124	1.59189	1.58802	1.58715	1.58683	1.58643	1.58632
19700	1.63168	1.61993	1.61506	1.61397	1.61357	1.61307	1.61293
20000	1.66337	1.64871	1.64264	1.64127	1.64077	1.64016	1.63999
20000	1.66337	1.64871	1.64264	1.64127	1.64077	1.64016	1.63999
20300	1.69647	1.67828	1.67075	1.66905	1.66844	1.66769	1.66748
20600	1.73110	1.70869	1.69941	1.69732	1.69656	1.69565	1.69540

PARTITION FUNCTION OF B II [Continued]

T K \ ΔE eV	.05	.10	.25	.50	1.00	2.00	3.00
20900	1.76745	1.74000	1.72863	1.72607	1.72514	1.72403	1.72373
21200	1.80570	1.77227	1.75842	1.75531	1.75417	1.75283	1.75247
21500	1.84606	1.80557	1.78881	1.78503	1.78366	1.78205	1.78162
21800	1.88878	1.83999	1.81979	1.81525	1.81359	1.81167	1.81116
22100	1.93412	1.87562	1.85142	1.84597	1.84398	1.84170	1.84110
22400	1.98235	1.91257	1.88369	1.87720	1.87483	1.87212	1.87142
22700	2.03381	1.95094	1.91666	1.90895	1.90614	1.90295	1.90212
23000	2.08883	1.99086	1.95034	1.94123	1.93791	1.93416	1.93416
23300	2.14778	2.03246	1.98477	1.97406	1.97014	1.96577	1.96465
23600	2.21107	2.07589	2.02000	2.00744	2.00286	1.99777	1.99648
23900	2.27913	2.12131	2.05606	2.04141	2.03606	2.03016	2.02867
24200	2.35245	2.16889	2.09301	2.07597	2.06975	2.06294	2.06123
24500	2.43151	2.21881	2.13089	2.11115	2.10395	2.09610	2.09415
24800	2.51685	2.27126	2.16976	2.14698	2.13866	2.12966	2.12743
25100	2.60905	2.32645	2.20967	2.18347	2.17390	2.16360	2.16107
25400	2.70871	2.38460	2.25069	2.22065	2.20969	2.19794	2.19508
25700	2.81648	2.44595	2.29288	2.25855	2.24602	2.23268	2.22944
26000	2.93304	2.51075	2.33631	2.29720	2.28293	2.26781	2.26416
26300	3.05909	2.57925	2.38107	2.33664	2.32043	2.30334	2.29924
26600	3.19541	2.65174	2.42721	2.37689	2.35853	2.33928	2.33469
26900	3.34277	2.72849	2.47483	2.41799	2.39726	2.37563	2.37049
27200	3.50200	2.80981	2.52401	2.45998	2.43664	2.41239	2.40666
27500	3.67397	2.89602	2.57485	2.50291	2.47668	2.44956	2.44319
27800	3.85958	2.98745	2.62742	2.54680	2.51740	2.48716	2.48009
28100	4.05976	3.08443	2.68184	2.59170	2.55884	2.52518	2.51735
28400	4.27550	3.18732	2.73820	2.63766	2.60101	2.56364	2.55499
28700	4.50780	3.29649	2.79660	2.68472	2.64394	2.60254	2.59300
29000	4.75770	3.41232	2.85716	2.73292	2.68766	2.64188	2.63138
29300	5.02628	3.53520	2.91998	2.78233	2.73218	2.68168	2.67014
29600	5.31467	3.66555	2.98518	2.82298	2.77754	2.72193	2.79929
29900	5.62399	3.80377	3.05288	2.88493	2.82376	2.76265	2.74881
30200	5.95544	3.95030	3.12319	2.93824	2.87088	2.80384	2.78873
30500	6.31022	4.10557	3.19625	2.99295	2.91892	2.84552	2.82904
30800	6.68958	4.27005	3.27218	3.04912	2.96790	2.88769	2.86974
31100	7.09478	4.44418	3.35111	3.10681	3.01787	2.93034	2.91085
31400	7.52713	4.62845	3.43318	3.16608	2.06885	2.97350	2.95235
31700	7.98795	4.82333	3.51851	3.22698	3.12087	3.01717	2.99426
32000	8.47859	5.02933	3.60726	3.28957	3.17397	3.06137	3.03659
32300	9.00043	5.24693	3.69955	3.35393	3.22817	3.10609	3.07932
32600	9.55488	5.47665	3.79553	3.42010	3.28351	3.15136	3.12248
32900	10.14335	5.71900	3.89535	3.48814	3.34002	3.19716	3.16606
33200	10.76730	5.97452	3.99915	3.55814	3.39774	3.24353	3.21007
33500	11.42820	6.24373	4.10708	3.63013	3.45669	3.29045	3.25451
33800	12.12752	6.52717	4.21930	3.70420	3.51691	3.33795	3.29938
34100	12.86676	6.82539	4.33595	3.78041	3.57844	3.38602	3.34470
34400	13.64846	7.13894	4.45719	3.85882	3.64131	3.43469	3.39046
34700	14.47113	7.46837	4.58317	3.93950	3.70555	3.48395	3.43667
35000	15.33934	7.81424	4.71405	4.02251	3.77120	3.53382	3.48333

FUNKCIJA PARTICIJE ZA ATOME B I I B II

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Sadržaj

U radu je proračunata funkcija particije za neutralni i jedanput ionizirani atom bora, u intervalu temperatura od 5000 do 35000 K. Uz starije podatke o energetskim nivoima[6-9], dovoljan su broj podataka za proračun dali tek noviji radovi[2-5]. Tablice su ispisane analogno tablicama Drawina i Felenboka[1], gdje je funkcija particije navedena u ovisnosti o temperaturi, te o sniženju energije ionizacije ΔE (izraženom u elektron-voltima) kao parametru.