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Tables of the Partition Functions for Iron, Fe I–Fe X

by

J. Halenka[1], and J. Madej[2,3]

[1] Institute of Physics, University of Opole, Oleska 48, 45–052 Opole, Poland
e-mail: halenka@uni.opole.pl
[2] Astronomical Observatory, University of Warsaw, Al. Ujazdowskie 4,
00-478 Warszawa, Poland
e-mail: jm@astrouw.edu.pl
[3] Copernicus Astronomical Center, Polish Academy of Sciences, Bartycka 18,
00-716 Warszawa, Poland

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ABSTRACT

We present extensive tables of the Atomic Partition Function for iron ions, Fe I–Fe X, and discuss details of the computational method. Partition functions are given in wide range of temperatures, 10^3 K $< T <$ 10^6 K, and lowering of ionization energy (0.001 eV $< LIE <$ 5.0 eV). Our APF take into account all energy levels predicted by quantum mechanics, including autoionization levels. The tables can be applied for the computations of model stellar atmospheres and theoretical spectra over all existing spectral and luminosity classes.

Our tables are available via Internet from Acta Astronomica Archive or *http://draco.uni.opole.pl/Halenka.html*.

Key words: *Atomic data – Plasmas – Stars: atmospheres*

1. Introduction

Iron is the most abundant and important heavy element in astrophysical plasmas. Due to its relatively high abundance in solar type composition and low ionization energy, iron ions are important contributors of free electrons in stellar atmospheres of population II at low and moderate effective temperatures (spectral types F and lower). In atmospheres of these types hydrogen and helium atoms remain almost perfectly neutral, and therefore iron donors of free electrons can be critically important for the populations and opacity of negative ions H^- and He^-, which in turn determine the whole atmospheric structure and visual/infrared spectra of these most numerous classes of stars.

Also on the opposite end of the Hertzsprung-Russell diagram, various ions of iron contribute to the stratification of monochromatic bound-free and line opacities in stellar atmospheres of the highest effective temperatures, including both main sequence and white dwarf stars. Highly ionized iron ions efficiently absorb extreme ultraviolet and X-ray photons, where the outgoing flux of radiation is most intense in these objects. Therefore iron plays a crucial role in determining the structure of atmospheres and appearance of the radiation spectra of the hottest stars.

Both the above examples show the importance of construction of the partition functions for various iron ions, which are internally homogeneous and can determine exactly populations of iron ions over very wide range of temperatures and electron concentrations. Our paper fulfills such a demand.

Values of the partition function U for a particular ion depend on gas temperature T, and the local electron concentration N_e. Temperature enters partition function by its definition (Griem 1964, Drawin and Felenbok 1965, Traving *et al.* 1966)

$$U(T,N_e) = \sum_{i=1}^{i_{\max}} g_i \exp(-E_i/kT) \qquad (1)$$

where the sum is taken over discrete energy levels of statistical weights i and excitation energies E_i. In vacuum ($N_e = 0$) the number of bound levels $i_{\max}$ is infinite, and therefore the above series diverges.

In real plasma, however, interaction between the atom of interest and surrounding free electrons and ions cause, that bound levels of very high excitation energies move to continuum and no longer contribute to the partition function. Therefore the series in Eq. (1) reduces to finite number of terms, and value of U is also finite and is strongly dependent on the electron concentration N_e. In general, the larger is N_e the lower is both number of bound energy levels $i_{\max}$ in Eq. (1), and the value of U.

There exist a large number of papers, which present tables of rather approximate (or even schematic) partition functions (APF) for elements, including few iron ions (Drawin and Felenbok 1965, Traving *et al.* 1966, Irwin 1981, for example). The latter paper presents fitting formulae for APF of Fe I–Fe III, for temperatures $T \leq 16\,000$ K. The widely used computer code Tlusty 195 for computations of NLTE model stellar atmospheres (Hubeny and Lanz 1992, 1995) contains FORTRAN subroutine computing APF of Fe IV–Fe IX by direct summation over all energy levels *observed* in these ions in 1971. Therefore the set of energy levels was not complete in TLUSTY195.

Quality of given tables of partition functions depends on (i) accuracy and completeness of energy levels included in Eq. (1), and (ii) reliability of the assumed theory of emitter-plasma interactions. Emitter-plasma interactions cause that the series in Eq. (1) is finite. Unfortunately, none of the currently existing theories describe correctly effects of charged particles in plasma on the atomic partition functions, *cf.* also Hummer and Mihalas (1988).

We have computed and present tables of the partition functions taking into account all energy levels predicted by quantum mechanics, including also levels lying above the so called *normal ionization energy* (autoionization levels). Moreover, our computations are more physically correct, since values of APF depend on both temperature T and electron concentration N_e. The latter is related to the lowering of ionization energy (LIE). The method of APF calculations is described in the following Section. This method was also presented in series of papers by Halenka and Grabowski (1977, 1984, 1986), Halenka (1988, 1989), and Madej *et al.* (1999). Paper by Halenka *et al.* (2001, hereafter Paper I) presented already extensive tables of APF for nickel, Ni I–Ni X, which were computed in the same way.

2. Computations of the Atomic Partition Functions

We have appended contribution to the Atomic Partition Function given by autoionizing levels. We replace the classical definition of APF, Eq. (1), by more realistic expression introduced by Halenka and Grabowski (1977) as follows

$$U^{(r)}(T,N_e) = \sum_{p=1}^{p_{\max}} \sum_{i=1}^{i(p)_{\max}} g_{pi}^{(r)} \exp(-E_{pi}^{(r)}/kT) = \sum_{p=1}^{p_{\max}} U_p^{(r)}(T,N_e). \qquad (2)$$

Here the set (pi) with the indices p and i (ordering of levels from the ground level upwards in energy scale) describes an eigenstate of the atom in the r-th ionization state. Index i represents three quantum numbers (nlj) of the optical electron, and p represents the quantum state of the atomic core. Index $i(p)_{max}$ is the number of all bound energy levels, $g_{pi}^{(r)}$ and $E_{pi}^{(r)}$ denote statistical weight and excitation energy of the i-th state, in the sequence based on the p-th parent level. Numbers $i(p)_{max}$ result from the inequality

$$E_{pi}^{(r)} \leq E_{p\infty}^{(r)} - \Delta E^{(r)} \qquad (3)$$

where $\Delta E^{(r)}$ denotes the lowering of the ionization energy LIE, and $E_{p\infty}^{(r)}$ is the ionization energy in the p-th level sequence. The latter quantity is equal to the sum

$$E_{p\infty}^{(r)} = E_{1\infty}^{(r)} + E_p^{(r+1)}. \qquad (4)$$

The quantity $E_p^{(r+1)}$ denotes the energy of the atomic core after ionization, $r \rightarrow r+1$. Index $p_{\max}$ is the number of different parent levels which can be realized in given physical conditions. The number $p_{\max}$ results from the inequality similar to Eq. (3), written for the $(r+1)$-th ionization state. Since for a fixed value of p the number k is assigned unambiguously, then the upper limit of $E_{p\infty}^{(r)}$ for the k-fold excitation can be written as follows. Numbers $k = 1,2,\ldots,Z-r$, where Z denotes the atomic number

$$E_{p\infty}^{(r)} \leq \sum_{s=1}^{k} E_{1\infty}^{(r+s-1)}. \qquad (5)$$

The above definition of *APF* requires, that for a fixed ionization state r the initial set of observed and calculated energy levels must be split into level sequences according to their attachment to different parent terms. Our initial set of levels was taken from catalogue of energy levels of iron ions from the CD-ROM by Kurucz (1994), which contained both the "observed" and computed energy levels (of the order 1000 for each ionization state r). We have also added to our *APF*'s contribution from many energy levels predicted by quantum mechanics, which were missed in CD-ROM by Kurucz. Exact description of the method of adding of missing levels was given by Halenka and Grabowski (1977, 1984).

Given term of a configuration with equivalent electrons usually belongs simultaneously to few level sequences defined by different parent terms. To calculate the contribution of a fixed term i to the partial *APF*, $U_p^{(r)}$ in Eq. (2), one must multiply the statistical weights of the i-th term by their coefficients of the fractional parentage G_{qi}, which were normalized to 1. We have assigned coefficients of the fractional parentage according to the well known procedure (*cf.* Slater 1960, Sobelman 1979):

$$G_{pi} \equiv G_{\alpha' L' S';\alpha LS} = (\alpha' L' S';\alpha LS)^2 / \sum{}' \alpha' L' S';\alpha LS)^2. \tag{6}$$

For a fixed ionization degree r, all level sequences were divided into three groups: $\alpha^{(r)}$, $\beta^{(r)}$, and $\gamma^{(r)}$.

Group $\alpha^{(r)}$ consists of level sequences numbered by $p = 1, 2, \ldots, p_1$, where all energy levels (energies and statistical weights) are known. Usually the total number of such level sequences does not exceed 20. In most cases these level sequences belong to the ground parent configuration. Their contribution to the *APF* is given by summation of terms in Eq. (2).

Group $\beta^{(r)}$ consists of level sequences, in which only part of energy levels are known, from $i = 1$ up $i_1(p)$. Number of such level sequences, $p = p_1 + 1, \ldots, p_2$, never exceeds one hundred. Contributions of $\beta^{(r)}$ level sequences to the *APF* is given by summation up to level $i_1(p)$. Remaining levels are included approximately, assuming their similarity to some of level sequence of the group $\alpha^{(r)}$, so called reference level sequence. Thus, for $p_1 < p \leq p_2$, values of $U_p^{(r)}$ can be calculated according to the relation:

$$\sum_{p \in term\ s} U_p^{(r)} = \sum_{p \in term\ s} \sum_{i=1}^{i_1(p)} g_{pi}^{(r)} \exp(-E_{pi}^{(r)}/kT) + \sum_{p \in term\ s} \Delta U_p^{(r)} \tag{7}$$

where

$$\sum_{p \in term\ s} \Delta U_p^{(r)} \simeq \sum_{p \in term\ q} \Delta U_p^{(r)} \frac{\sum_{p \in term\ s} g_p^{(r+1)} \exp(-E_{pi}^{(r+1)}/kT)}{\sum_{p \in term\ q} g_p^{(r+1)} \exp(-E_{pi}^{(r+1)}/kT)} \tag{7$'$}$$

and

$$g_{pi} = (2J_{pi} + 1) G_{pi}.$$

Here q $(q \le p_1)$ represents a reference level sequence.

Group $\gamma^{(r)}$ is the set of level sequences, in which no levels are known. Their share in the *APF* can be estimated from the expression

$$\sum_{p_2+1}^{p_{\max}} U_p^{(r)} = \frac{\sum\limits_{p \in term\ q} U_p^{(r)}}{\sum\limits_{p \in term\ q} g_p^{(r+1)} \exp(-E_{pi}^{(r+1)}/kT)} \times$$
$$\times \left[U^{(r+1)} - \sum_{p=1}^{p_2} g_p^{(r+1)} \exp(-E_{pi}^{(r+1)}/kT) \right]. \qquad (8)$$

The relation Eq. (7') is strictly valid if, at a fixed quantum number J of the optical electron, change $s \to q$ of the state of the atomic core does not alter the electron-core interaction energy. In such a case energy levels of the s sequence are shifted as a whole relatively to q sequence by energy $|E_s^{(r+1)} - E_q^{(r+1)}|$, and the statistical weighs satisfy the relation $g_s^{(r)}/g_q^{(r)} = g_s^{(r+1)}/g_s^{(r+1)}$.

The above condition is never strictly realized. However, the error introduced into $U_p^{(r)}$ by the Eq. (7') reaches minimum when the maximum bound energies in both considered level sequences (s and q) reach similar values. It should be noted that values of $U^{(r)}$ are of physical interest only in such range of temperatures T, when $E_{p\infty}^{(r)}/kT \gg 1$. Since for $p > p_1$ we have $E_{pi}^{(r)} \ge E_{1\infty}^{(r)}$ (except for few of the lowest levels), then the error contributed by $\Delta U_p^{(r)}$ to $U^{(e)}$ in Eq. (7') is always small.

3. Results

We have computed *APF* for Fe I–Fe X ions according to above procedure. Exemplary results shown in Fig. 1, which displays run of our *APF* for Fe IV and temperatures corresponding to atmospheres of hot white dwarf stars, for various values of *LIE* taken as free parameter (solid lines). Numerical values of log *APF* for Fe IV are also listed in Table 1. In Fig. 1 we have appended run of partition functions computed on the basis of the observed levels only (single dashed line). One can easily note, that our recommended partition functions are significantly larger than the latter functions, and apparently tend to diverge at any fixed T and $N_e \to 0$.

Partition functions for iron are arranged in 10 ASCII tables, where each table corresponds to a single ion, which is identical with the organization of Ni I–Ni X partition functions of Paper I. Full set of these data is available from Acta Astronomica Archive,

http://www.astrouw.edu.pl/∼acta/acta.html

or

Table 1

Atomic partition functions for Fe IV (decimal logarithms)

	Lowering of ionization energy (eV)								
T (K)	0.001	0.003	0.010	0.030	0.100	0.300	1.000	3.000	5.000
1000	0.7782	0.7782	0.7782	0.7782	0.7782	0.7782	0.7782	0.7782	0.7782
3000	0.7782	0.7782	0.7782	0.7782	0.7782	0.7782	0.7782	0.7782	0.7782
6000	0.7800	0.7800	0.7800	0.7800	0.7800	0.7800	0.7800	0.7800	0.7800
8000	0.7905	0.7905	0.7905	0.7905	0.7905	0.7905	0.7905	0.7905	0.7905
10000	0.8196	0.8196	0.8196	0.8196	0.8196	0.8196	0.8196	0.8196	0.8196
12000	0.8709	0.8709	0.8709	0.8709	0.8709	0.8709	0.8709	0.8709	0.8709
14000	0.9401	0.9401	0.9401	0.9401	0.9401	0.9401	0.9401	0.9401	0.9401
16000	1.0193	1.0193	1.0193	1.0193	1.0193	1.0193	1.0193	1.0193	1.0193
18000	1.1013	1.1013	1.1013	1.1013	1.1013	1.1013	1.1013	1.1013	1.1013
20000	1.1812	1.1812	1.1812	1.1812	1.1812	1.1812	1.1812	1.1812	1.1812
23000	1.2924	1.2923	1.2923	1.2923	1.2923	1.2923	1.2923	1.2923	1.2923
26000	1.3924	1.3912	1.3910	1.3909	1.3909	1.3909	1.3909	1.3909	1.3909
30000	1.5382	1.5110	1.5054	1.5045	1.5043	1.5043	1.5043	1.5043	1.5043
35000	2.0191	1.7321	1.6428	1.6268	1.6236	1.6230	1.6229	1.6228	1.6228
40000	2.8838	2.2692	1.8725	1.7563	1.7293	1.7244	1.7234	1.7231	1.7231
50000	4.8825	3.7789	2.8867	2.3089	2.0008	1.9172	1.8978	1.8937	1.8928
55000	6.0263	4.6774	3.5030	2.7413	2.2318	2.0372	1.9846	1.9734	1.9709
60000	7.1605	5.6211	4.1928	3.2122	2.5295	2.1919	2.0796	2.0541	2.0485
65000	8.3485	6.5641	4.9319	3.7250	2.8702	2.3851	2.1878	2.1385	2.1277
70000	9.5500	7.5398	5.6795	4.2795	3.2435	2.6112	2.3122	2.2285	2.2100
75000	10.7275	8.5356	6.4405	4.8545	3.6478	2.8634	2.4534	2.3253	2.2963
80000	11.9105	9.5197	7.2226	5.4379	4.0762	3.1376	2.6104	2.4292	2.3872
85000	13.0986	10.4993	8.0111	6.0324	4.5190	3.4316	2.7817	2.5404	2.4830
90000	14.2644	11.4852	8.7950	6.6392	4.9713	3.7422	2.9663	2.6588	2.5838
95000	15.4087	12.4659	9.5781	7.2521	5.4327	4.0657	3.1630	2.7842	2.6898
100000	16.5444	13.4307	10.3642	7.8658	5.9029	4.3994	3.3709	2.9164	2.8009
110000	18.7507	15.3297	11.9257	9.0961	6.8602	5.0922	3.8156	3.2007	3.0392
120000	20.8490	17.1802	13.4597	10.3301	7.8285	5.8128	4.2928	3.5104	3.2987
130000	22.9556	18.9711	14.9712	11.5536	8.8050	6.5517	4.7965	3.8434	3.5788
140000	25.0807	20.7632	16.4512	12.7658	9.7829	7.3023	5.3206	4.1971	3.8777
150000	27.2496	22.5661	17.9197	13.9647	10.7566	8.0593	5.8588	4.5677	4.1925
160000	29.4830	24.3955	19.3919	15.1508	11.7248	8.8172	6.4055	4.9509	4.5196
170000	31.6978	26.2770	20.8733	16.3328	12.6870	9.5716	6.9562	5.3423	4.8550
180000	33.7774	28.1713	22.3837	17.5168	13.6449	10.3208	7.5074	5.7380	5.1951
190000	35.6762	29.9913	23.9277	18.7097	14.6030	11.0649	8.0562	6.1350	5.5370
200000	37.3981	31.6822	25.4660	19.9211	15.5653	11.8052	8.6013	6.5312	5.8786
220000	40.3846	34.6508	28.3275	22.3775	17.5068	13.2836	9.6784	7.3161	6.5547
230000	41.6858	35.9496	29.6102	23.5702	18.4789	14.0256	10.2115	7.7035	6.8878
240000	42.8797	37.1423	30.7949	24.7054	19.4410	14.7699	10.7423	8.0874	7.2170
250000	43.9790	38.2410	31.8893	25.7725	20.3818	15.5143	11.2714	8.4679	7.5423
265000	45.4738	39.7353	33.3807	27.2432	21.7311	16.6222	12.0631	9.0329	8.0230
280000	46.8098	41.0712	34.7152	28.5683	22.9870	17.7032	12.8514	9.5917	8.4957
300000	48.3852	42.6465	36.2898	30.1371	24.5059	19.0727	13.8900	10.3277	9.1143
325000	50.0843	44.3456	37.9885	31.8330	26.1703	20.6348	15.1470	11.2310	9.8692
350000	51.5429	45.8042	39.4471	33.2904	27.6108	22.0214	16.3308	12.1085	10.6025
375000	52.8089	47.0702	40.7131	34.5559	28.8658	23.2457	17.4230	12.9507	11.3103
400000	53.9183	48.1796	41.8225	35.6651	29.9677	24.3286	18.4181	13.7487	11.9882
425000	54.8985	49.1599	42.8028	36.6453	30.9424	25.2905	19.3199	14.4973	12.6323
450000	55.7710	50.0324	43.6754	37.5178	31.8106	26.1496	20.1359	15.1940	13.2401
475000	56.5528	50.8141	44.4572	38.2996	32.5888	26.9209	20.8752	15.8397	13.8104
500000	57.2572	51.5186	45.1617	39.0041	33.2903	27.6170	21.5466	16.4365	14.3438
525000	57.8954	52.1568	45.8000	39.6424	33.9259	28.2483	22.1583	16.9877	14.8414
550000	58.4763	52.7378	46.3809	40.2233	34.5045	28.8233	22.7174	17.4970	15.3051
600000	59.4947	53.7562	47.3994	41.2419	35.5191	29.8322	23.7017	18.4045	16.1400
650000	60.3585	54.6199	48.2633	42.1058	36.3797	30.6884	24.5398	19.1861	16.8668
700000	61.1004	55.3619	49.0053	42.8479	37.1191	31.4243	25.2616	19.8645	17.5026
750000	61.7448	56.0064	49.6498	43.4924	37.7613	32.0636	25.8896	20.4580	18.0620
800000	62.3098	56.5713	50.2148	44.0574	38.3243	32.6242	26.4409	20.9812	18.5573
850000	62.8092	57.0708	50.7143	44.5569	38.8221	33.1199	26.9287	21.4455	18.9984
900000	63.2539	57.5155	51.1590	45.0017	39.2653	33.5613	27.3633	21.8603	19.3935
950000	63.6524	57.9140	51.5576	45.4003	39.6625	33.9569	27.7531	22.2330	19.7493
1000000	64.0117	58.2733	51.9168	45.7596	40.0206	34.3136	28.1046	22.5696	20.0712

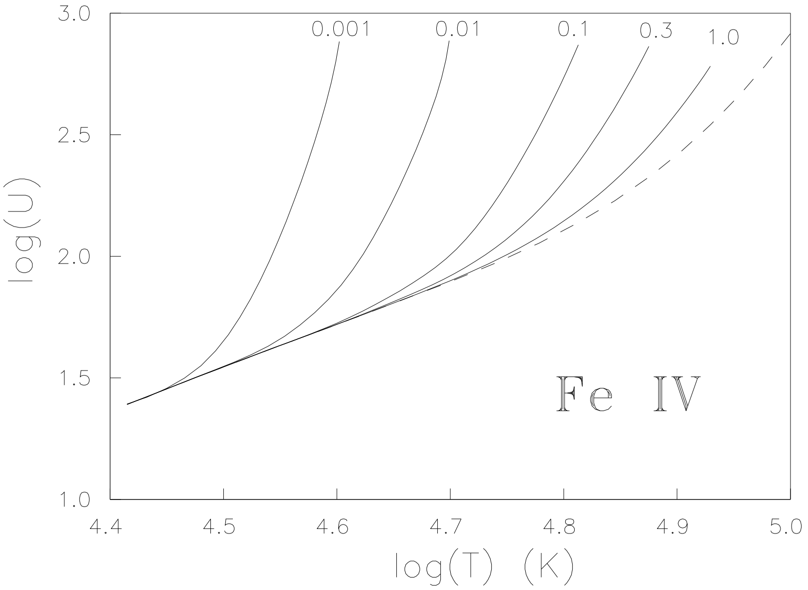

Fig. 1. Run of partition functions of Fe IV as function of gas temperature T and various parameters LIE. Solid lines represent our recommended results, whereas dashed line represents partition function computed from the observed levels only.

http://draco.uni.opole.pl/Halenka.html

Entries of tables are decimal logarithms of the APF. They are tabulated at 62 discrete temperatures, spaced at nonequidistant intervals, $10^3 \leq T \leq 10^6$ K, and at 9 arbitrarily assumed values of the lowering of ionization energy (LIE = 0.001, 0.003, 0.010, 0.030, 0.100, 0.300, 1.000, 3.000, and 5.000 eV). Both T and LIE points remain identical in all 10 tables of APF, to ensure homogeneity of the data and compatibility with Paper I.

Very wide range of both parameters T and LIE assumed in our tables ensures, that they cover practically all the conditions expected in stellar atmospheres of any type, reaching from the coldest dwarfs up to the hottest accreting white dwarf stars.

Tables discussed in this paper are based on the most complete set of energy levels actually available for iron ions. Moreover, our partition functions are sensitive to plasma interactions, since they strongly depend on the lowering of ionization energy. Our APF tend to diverge for the lowering of ionization energy approaching zero, and are perfectly compatible with the APF for nickel ions (*cf.* Paper I).

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