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**CALCULATIONS OF ASTROPHYSICAL
PARTITION FUNCTIONS**

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CALCULATIONS OF ASTROPHYSICAL PARTITION FUNCTIONS

SUMMARY

This report outlines a method for the calculation of the internal energy partition function of an atom or ion immersed in a plasma. The influence of the surrounding plasma on the atom or ion is considered by including a probability function P_i in the sum over the energy states:

$$\text{partition function } U = \sum_{i=1}^{\infty} g_i P_i e^{-\chi_i/kT}$$

In this expression g_i is the statistical weight of the i th level with excitation energy χ_i , T is the absolute temperature, and k is the Boltzmann constant. The function P_i denotes the probability that an atom or ion in the i th energy level is not perturbed by surrounding ions, and it is a function of the temperature and electron pressure of the plasma. The calculation for the partition function U is done in three steps. The first is an actual summation over all levels belonging to principal quantum numbers for which the energy levels are completely tabulated; the second step is a summation through principal quantum number 15, assuming hydrogenic levels. In the last step the remaining sum is approximated by an integral and all levels χ_i are replaced by the ionization potential. The contributions of parent configurations other than the series limit are included and the final equation is written in a form that explicitly shows the effect of higher parent terms in the calculations.

Numerical results are presented for four different species at several temperatures and pressures; these are compared with calculations of other authors. In the case of Al II (Mg I isoelectronic sequence), which has two parent configurations, the error incurred by considering only the main parent term in the calculations is clearly demonstrated.

INTRODUCTION

To fully interpret the experimental data obtained from a magnetograph system, the theory for the formation of a Zeeman-sensitive absorption line in a magnetic field must be investigated. Moe [1] has shown how the radiative transfer equations for polarized light, as derived by Unno [2], can be numerically integrated using any desired atmospheric model. In his derivation Moe has made the assumption of local thermodynamic equilibrium so that the rate equations and transfer equations are uncoupled and the level populations are governed by the Saha-Boltzmann equations. These latter equations require the calculation of internal energy partition functions for atoms and ions, taking into consideration their dependence on the local temperature and electron pressure of the surrounding plasma. This report outlines the program that was developed in order that partition functions could be calculated for any atom or ion, using any desired atmospheric model.

PARTITION FUNCTIONS OF ATOMS AND IONS IN A PLASMA

Partition functions enter into astrophysical calculations in the determination of atomic level populations through the Saha and Boltzmann equations. In particular, one must calculate the internal energy partition function for atoms or ions with all energies measured relative to the ground state:

$$U = \sum_{i=1}^{\infty} g_i e^{-\chi_i/kT} \quad (1)$$

Here g_i is the statistical weight of the i th level, χ_i is the excitation energy of the i th level, T is the absolute temperature, and k is the Boltzmann constant. For an isolated atom or ion, the partition function is divergent because of the combining factors of an infinite number of levels and a series limit. However, when an atom (or ion) is immersed in a plasma, the higher levels that were bound states in the isolated atom become continuum states because of the interaction between the atom and neighboring ions. Thus the number of bound levels is finite and the partition function sum is convergent. This concept can be analytically expressed as a probability function, P_i , which denotes the probability that an atom in the i th energy level is not

perturbed by the surrounding plasma. For the lowest-lying levels, P_i is one; for the higher levels, the energy of the states decreases, and the optical electrons are more influenced by perturbations from surrounding ions on the potential field in which they move so that P_i decreases. Finally, when the interaction energy is comparable to the ionization energy of the bound optical electrons, the state is destroyed and P_i is zero. The partition function can thus be written

$$U = \sum_{i=1}^{\infty} g_i P_i e^{-\chi_i/kT} \quad (2)$$

The determination of the probability P_i has been approached in several ways. The method outlined below is due to Unsöld [3]. A different approach to the problem is to consider the reduction of the ionization limit as outlined by Griem [4]. Basically, Unsöld considers P_i to be given by the probability that the nearest neighboring ion is beyond a critical distance R_c :

$$P_i = e^{-\frac{4\pi}{3} N_o R_c^3}, \quad (3)$$

where N_o is the number density of perturbing ions. For singly ionized perturbers, N_o equals the number density of free electrons N_e ; in general for a perturbing ion of charge Z' ,

$$Z' N_o = N_e = P_e/kT, \quad (4)$$

where P_e is the electron pressure.

Following the discussion of Pecker and Schatzman [5], R_c is that separation of the perturbing ion and atom at which the maximum potential energy of the optical electron in the resulting field of the atom and ion equals the ionization energy of the electron in its orbit.

From Figure 1, with R and r fixed, one can see that the potential energy of the electron will be greatest along the line of separation R between the atom and perturber. Thus,

$$E_P = -\frac{Z^2 e}{r} - \frac{Z'^2 e}{\rho} \quad , \quad (5)$$

where $\rho + r = R$. The effective charge of the atom minus the optical electron is denoted by Z_e . If we maximize

E_P under the constraint that

$\rho + r = R$, with R fixed, there results:

$$\frac{Z}{r_1^2} = \frac{Z'}{\rho_1^2} \quad , \quad (6)$$

Figure 1. Schematic diagram showing the relative separations of atom, ion and electron.

where r_1 and ρ_1 are the respective values of r and ρ at which E_P is a maximum. Thus,

$$\left(E_P\right)_{\text{maximum}} = -\frac{Z^2 e}{r_1} - \frac{Z'^2 e}{\rho_1} \quad (7)$$

with $\frac{r_1}{\rho_1} = \sqrt{\frac{Z}{Z'}}$.

Then R_c is the separation distance at which this maximum potential energy equals the ionization energy of the optical electron with shell number n_i :

$$-\frac{Z e^2}{r_1} - \frac{Z' e^2}{\rho_1} = -\frac{h c Ry Z^2}{n_i^2} \quad . \quad (8)$$

In this expression hydrogenic levels have been assumed for the optical electron; Ry is the Rydberg constant, h is Planck's constant and c is the velocity of light. Using the relation $R_c = r_1 + \rho_1$ and equation (6), the expression for R_c becomes

$$R_c = n_i^2 \left[\frac{e^2(Z + Z' + 2\sqrt{Z Z'})}{h c Ry Z^2} \right] \quad . \quad (9)$$

The probability function P_i is now written

$$P_i = e^{-C(Z) P_e \theta n_i^6} \quad (10)$$

where $\theta \equiv \frac{5040}{T}$. The constants $C(Z)$ are tabulated in Aller [6].

REDUCTION OF THE PARTITION FUNCTION EQUATION FOR PRACTICAL CALCULATIONS

For an atom (or ion), the partition function is to be calculated from the expression

$$U = \sum_{i=1}^{\infty} g_i e^{-C(Z) P_e \theta n_i^6} e^{-\chi_i/kT} \quad (11)$$

The energy states χ_i are tabulated in tables of atomic energy levels [7], but, for most atoms, these tables are incomplete, with only levels of the lower orbital angular momentum configurations being known. Following the approach outlined by Aller, Elste and Jugaku [8], U is written as the sum of two parts:

$$U = U_0 + U_1 \quad (12)$$

If the atomic energy level tables become incomplete at principal quantum number $n_i = m$,

$$U_0 = \sum_{i=1}^{n_i=(m-1)} g_i P_i e^{-\chi_i/kT} \quad (13)$$

with $g_i = 2 J_i + 1$. In the tables of Reference 7, the energy levels are expressed as wave numbers so it is convenient to write

$\chi_i/kT = (2.8548 \times 10^{-4}) \theta \tilde{\nu}_i \equiv c_1 \theta \tilde{\nu}_i$. The term U_1 is the remaining summation over higher levels of which wave numbers are incompletely tabulated. To include all the states of these higher levels, it seems best to

assume hydrogenic structure for the levels and perform the sum, rather than use the tabulated levels and risk omission of states with high statistical weights. Accordingly,

$$U_1 = \sum_{n_i=m}^{\infty} g_i P_i e^{-c_1 \theta \left[\tilde{\nu}_L - Ry \frac{Z^2}{n_i^2} \right]}, \quad (14)$$

where $Ry = 109\,678.758 \text{ cm}^{-1}$, $Z = 1$ for neutral atoms, $Z = 2$ for singly ionized atoms, etc., and $\tilde{\nu}_L$ is the wave number limit of the atom or ion. The statistical weight g_i of a hydrogen-like system consisting of a "running" electron with outer shell number n_i added to a "parent configuration" with a multiplicity of states $(2S + 1)(2L + 1)$ is given by

$$g_i = 2 n_i^2 (2S + 1) (2L + 1). \quad (15)$$

The quantum numbers S and L refer to the parent configuration of the atom (or ion). Usually the term "parent configuration" refers to the ground state of the next higher ionization stage; however, some systems have more than one parent term and this must be considered in the summation of U_1 . Suppose there are N parent terms listed in the tables of predicted terms. Then

$$U_1 = \sum_{j=1}^N \sum_{n_i=m}^{\infty} (g_i)_j P_i e^{-c_1 \theta \left[(\tilde{\nu}_L)_j - Ry \frac{Z^2}{n_i^2} \right]}. \quad (16)$$

The wave number limits of the higher parent terms can be written in terms of the series limit $\tilde{\nu}_L$:

$$(\tilde{\nu}_L)_j = \tilde{\nu}_L + (\Delta\tilde{\nu})_j,$$

where $(\Delta\tilde{\nu})_j$ refers to the listed wave number of the j th parent configuration in the tables for the next higher ionization stage. The statistical weights $(g_i)_j$ can be written as

$$(g_i)_j = 2 n_i^2 (2 S_j + 1) (2 L_j + 1) .$$

Then equation (16) becomes

$$U_1 = \left[2 (2 S_1 + 1) (2 L_1 + 1) \sum_{n_i=m}^{\infty} n_i^2 P_i e^{-c_1 \theta \left(\tilde{\nu}_L - Ry \frac{Z^2}{n_i^2} \right)} \right] \times \left[1 + \sum_{j=2}^N \frac{(2 S_j + 1) (2 L_j + 1)}{(2 S_1 + 1) (2 L_1 + 1)} e^{-c_1 \theta (\Delta \tilde{\nu})_j} \right] . \quad (17)$$

The last term in brackets in equation (17) represents the contribution of all parent terms other than the series limit term (with quantum numbers S_1 and L_1). This contribution is independent of P_e and can be easily evaluated for a given range of θ to determine the importance of higher parent terms in the calculation of U_1 .

The summation over the hydrogenic levels in U_1 is performed through $n_i = 15$ (U_{11}); the remaining sum (U_{12}) is approximated by an integral where the following assumption is also made:

$$\tilde{\nu}_L - Ry \frac{Z^2}{n_i^2} \approx \tilde{\nu}_L , \text{ for } n_i > 15.$$

Thus the expression for U_{12} can be written as

$$U_{12} = 2 (2 S_1 + 1) (2 L_1 + 1) 10^{-\chi_L \theta} \int_{n=16}^{\infty} n^2 e^{-[C(Z) P_e \theta] n^6} dn , \quad (18)$$

where χ_L is expressed in eV. With the substitution

$$n = y^{1/3} [C(Z) P_e \theta]^{-1/6} ,$$

there results

$$U_{12} = \frac{2(2S_1+1)(2L_1+1)}{3\sqrt{C(Z)P_e^\theta}} 10^{-\chi_L\theta} \int_{y_0}^{\infty} e^{-y^2} dy, \quad (19)$$

where $y_0 = 16^3 \sqrt{C(Z)P_e^\theta}$. The final result for the total partition function becomes:

$$\begin{aligned} U = & \sum_{i=1}^{n_i=(m-1)} (2J_i+1) P_i e^{-c_1\theta \tilde{\nu}_i} + \left[2(2S_1+1)(2L_1+1) \right. \\ & \times \sum_{n_i=m}^{15} n_i^2 P_i e^{-c_1\theta \left(\tilde{\nu}_L - Ry \frac{Z^2}{n_i^2} \right)} + \frac{\frac{\sqrt{\pi}}{3}}{\sqrt{C(Z)P_e^\theta}} (2S_1+1) \\ & \left. \times (2L_1+1) 10^{-\chi_L\theta} \operatorname{Erfc}(y_0) \right] \left[1 \right. \\ & \left. + \sum_{j=2}^N \frac{(2S_j+1)(2L_j+1)}{(2S_1+1)(2L_1+1)} e^{-c_1\theta(\Delta\tilde{\nu})_j} \right], \quad (20) \end{aligned}$$

with $P_i = e^{-C(Z)P_e^\theta n_i^6}$. The error function can be evaluated from the expansion

$$\operatorname{Erfc}(y_0) = e^{-y_0^2} (a_1 t + a_2 t^2 + a_3 t^3 + a_4 t^4 + a_5 t^5),$$

where $t = [1 + (0.3275911) y_0]^{-1}$, and

$$\begin{aligned} a_1 &= 0.254829592, \\ a_2 &= -0.284496736, \\ a_3 &= 1.421413741, \\ a_4 &= -1.453152027, \\ a_5 &= 1.061405429. \end{aligned}$$

NUMERICAL CALCULATIONS

A FORTRAN program has been written specifically for the calculation of Fe I and Fe II partition functions, which occur in the analysis of the formation of the Fe I 5250.2-Å line in a magnetic field, following the approach of Moe [1]. The program was designed to be flexible enough to be adapted to other atoms or ions, as well as to be able to handle various photospheric and sunspot models. The program is divided into three parts corresponding to the calculations of U_0 , U_{11} and U_{12} .

In the calculation of U_0 , all the wave numbers ($\tilde{\nu}_i$), statistical weights ($2J_i + 1$), and shell numbers (n_i) must be read into the program. The shell number m at which the wave number tables become incomplete can be determined by a comparison of the tables of the observed and predicted terms. If the observed terms are almost complete for a given shell number, the missing states can be estimated from corresponding terms of other members of the isoelectronic sequence. Or, if the missing states have small statistical weights and correspond to higher wave numbers, they may be neglected in the sum. The calculations for U_{11} and U_{12} are straightforward.

To check out the program, partition functions were calculated for four different species, ranging from simple-series spectra to complex spectra: Al III (Na I isoelectronic sequence), Al II (Mg I sequence, two parent configurations), Fe I (Fe I sequence, 19 parent configurations), and Fe II (Mn I sequence, 24 parent configurations).

Al III

For Al III, the tables of wave numbers are complete from the $3s^2S$ through the $6h^2H^\circ$ configuration; the sum in U_{11} is thus started at $n_i = 7$.

In compiling the known levels, each substate was considered separately for the three lowest levels. The parent configuration of Al III is a 1S_0 state, which indicates a parent multiplicity of one. The partition functions for Al III were calculated for various electron pressures at the temperature $\theta = 0.14$; the results are listed in Table 1 together with Al III partition functions calculated by Aller, Elste and Jugaku [6, 8].

TABLE 1. COMPUTED PARTITION FUNCTIONS FOR Al III

θ	Log P _e	Al III U	Al III U ^a
0.14	2.0	13.086	13.18
0.14	3.0	6.16	6.17
0.14	4.0	3.97	3.98

a. [6,8].

Al II

For singly ionized aluminum, Al II, the calculations are more complex because of the presence of two parent configurations in the table of observed terms: 2S and $^2P^0$. For the $n_i = 3$ shell number of the optical electron, there are four missing terms: the 1S term of the $3p^2$ configuration and the $^1P^0$, $^1D^0$ and $^1F^0$ terms of the $3p(^2P^0)3d'$ configuration. Wave numbers were estimated for these levels using the wave numbers of corresponding terms of Si III and P IV.

Because of the existence of the two parent terms, the partition function was evaluated twice, first considering only contributions for $n_i \geq 4$ from the levels of terms belonging to the 2S parent configuration, and then considering contributions of both parent configurations. For the first case of the 2S parent term alone, the observed terms are complete through shell number five so that the sum U_{11} was begun at $n_i = 6$. The substates of the first seven terms of U_0 were summed separately; thereafter the terms were grouped as single levels. The multiplicity $(2S + 1)(2L + 1)$ for the series limit 2S is 2. The resulting values for the partition function calculated in this manner are listed in Table 2 as $U(^2S)$.

TABLE 2. COMPUTED PARTITION FUNCTIONS FOR Al II

θ	Log P _e	U(2S)	U($^2S, ^2P^0$)	U ^a
0.14	2.0	213.2	285.7	213.8
0.14	3.0	72.2	95.6	72.4
0.14	4.0	26.3	33.7	26.9

a. [6,8].

When the contributions of both parent terms were considered, the sum in U_{11} was initiated at $n_i = 4$ since the observed terms of the ${}^2P^0$ parent configurations are very incomplete for $n_i > 3$. The partition function thus takes the form

$$\begin{aligned}
 U = & \sum_{n_i=3} (2J_i + 1) P_i e^{-c_1 \theta \tilde{\nu}_i} \left[2(2S_1 + 1)(2L_1 + 1) \sum_{n_i=4}^{15} n_i^2 \right. \\
 & \times P_i e^{-c_1 \theta \left(\tilde{\nu}_L - Ry \frac{Z^2}{n_i^2} \right) + \frac{\sqrt{\pi}}{3} \text{Erfc}(y_0) (2S_1 + 1)(2L_1 + 1) 10^{-\chi_L \theta}} \\
 & \left. \times \left[1 + \frac{(2S_2 + 1)(2L_2 + 1)}{(2S_1 + 1)(2L_1 + 1)} e^{-c_1 \theta \Delta \tilde{\nu}_2} \right] \right] \quad (21)
 \end{aligned}$$

For Al II, $\Delta \tilde{\nu}_2 \approx 53\,860 \text{ cm}^{-1}$ so that

$$\frac{(2S_2 + 1)(2L_2 + 1)}{(2S_1 + 1)(2L_1 + 1)} e^{-c_1 \theta \Delta \tilde{\nu}_2} = 3 e^{-15.376 \theta} \quad ; \text{ for } \theta = 0.14, \text{ this}$$

contributes a factor of 0.35 more to $[U_{11} + U_{12}]$. Numerical results using equation (21) are presented in Table 2 under the heading $U({}^2S, {}^2P^0)$. The last column represents data published by Aller, Elste and Jugaku [6, 8]. The effect of contributions from other parent terms can be clearly seen.

Fe I

The Fe I and Fe II partition function programs were initiated to calculate the populations of the lower level of the Fe I 5250.2 Å transition for various photospheric and sunspot models for which $0.4 \lesssim \theta \lesssim 1.9$.

Thus the effects of extremely high temperatures have been ignored. For Fe I, the sum U_0 included the $3d^6 4s^2$ and $3d^8$ levels plus all listed terms for which the active electron had a shell number $n_i = 4$. Missing states in the $3d^8$ configuration were estimated from similar terms in Co II and Ni III and from similar terms in members of the Ca I isoelectronic sequence, assuming a similarity between the $3d^8$ and $3d^2$ configurations. The missing

$3d^6 4s^2$ states were estimated from known wave numbers of tabulated members of that configuration. Missing levels for the $n_1 = 4$ shell number were numerous and no attempt was made to estimate them; rather, for a representative θ and P_e , their total contribution to the partition function was estimated, using hydrogenic levels, and found to be $\approx 1.0 \times 10^{-4}$. Therefore, no corrections were deemed necessary for them and the U_{11} sum was initiated at $n_1 = 5$. For both U_{11} and U_{12} , only the series limit configuration a 6D was considered as a parent term, although 19 actual parent terms exist. The effect of omitting these other parent configurations can be determined from the last term in brackets in equation (17). For a representative temperature for the solar photosphere, $\theta = 0.9705$, this term has the value $(1 + 0.63)$. However, for the a 6D parent term alone $(U_{11} + U_{12}) = 0.016$ (assuming $P_e = 3.554$ dynes/cm²). Thus all parent terms contribute a value of 0.026 to the total partition function. But at this temperature and pressure, $U_0 = 28.486$, so that it seems justified to consider only the a 6D parent term for photospheric and sunspot models; the contribution of the other 18 parent terms is insignificant, percentage wise. Table 3 compares the results of the computer program with tabulated values of Müller and Mutschlechner [9].

Fe II

From the tables of observed and predicted terms for Fe II, it can be seen that the $3d^7$ configuration is complete. Most of the remaining tabulated levels belong to $3d^5 4s^2$ or $3d^6$ (parent) $4x$ configurations ($x = s, p, d, f$), which are incomplete. Numerical estimates for $\theta = 1.00$ and $P_e = 2.5$ dynes/cm² indicate that all missing levels of the $3d^5 4s^2$ configuration would contribute $\approx 2.5 \times 10^{-3}$ to the partition function. Similar estimates for all other missing states with outer shell number $n_1 = 4$ indicate their total contribution would be less than 1.3×10^{-3} . Consequently the U_{11} sum was begun at $n_1 = 5$ and the U_0 sum included all listed levels with outer shell number $n_1 \leq 4$. In the calculations for U_{11} and U_{12} , only the main parent term a 5D was used; contributions of the other parent configurations are small at the temperatures considered because of the large wave number gap between the a 5D ground-state term ($\tilde{\nu} \approx 1027$ cm⁻¹) and the next lowest term, a 3P ($\tilde{\nu} \approx 20\,000$ cm⁻¹), in the Fe III level structure. The term in equation (17) that represents the contributions of other parent terms to

TABLE 3. PARTITION FUNCTION OF NEUTRAL IRON AS A FUNCTION OF TEMPERATURE AND ELECTRON PRESSURE

Log τ_0	θ^a	P_e	U	U^b
-3.6	1.0944	0.1323	26.465	26.430
-3.4	1.0938	0.1647	26.472	26.438
-3.2	1.0933	0.2044	26.478	26.444
-2.8	1.0913	0.3150	26.505	26.471
-2.4	1.0864	0.4882	26.572	26.539
-2.0	1.0748	0.7733	26.736	26.703
-1.6	1.0480	1.3070	27.138	27.103
-1.2	0.9990	2.4800	27.961	27.921
-1.0	0.9705	3.5540	28.502	28.457
-0.8	0.9400	5.3040	29.140	29.089
-0.4	0.8703	14.790	30.888	30.813
0	0.7835	62.450	33.868	33.723
0.4	0.6845	356.30	39.129	38.760
0.8	0.5688	2788.0	50.538	49.195
1.2	0.4365	26 780	82.113	75.980

a. $\theta \equiv 5040/T$

b. [9].

sum $U_{11} + U_{12}$ can easily be shown to be ≈ 0.01 for $\theta = 0.9705$ and $P_e = 3.554$ dynes/cm²; the a^5D term itself contributes practically nothing to the partition function at this θ and P_e so, again, the neglect of these other terms is justified. Sample calculations from the computer program are given in Table 4 along with values from the paper of Müller and Mutschlecner [9].

CONCLUSION

In conclusion, it should be emphasized that for higher temperatures the contributions of all parent terms should be carefully examined. In a paper by Traving, Baschek and Holweger [10], these effects have been considered in the calculations of partition functions for atoms and ions of astrophysical interest. The resulting partition functions are presented in polynomial form for easy machine calculations, eliminating the necessity of reading the tabulated energy levels into the program.

TABLE 4. PARTITION FUNCTION OF SINGLY IONIZED IRON AS A FUNCTION OF TEMPERATURE AND ELECTRON PRESSURE

Log τ_0	θ^a	P_e	U	U^b
-3.6	1.0944	0.1323	41.765	41.760
-3.4	1.0938	0.1647	41.775	41.771
-3.2	1.0933	0.2044	41.784	41.780
-2.8	1.0913	0.3150	41.820	41.816
-2.4	1.0864	0.4882	41.907	41.903
-2.0	1.0748	0.7733	42.118	42.114
-1.6	1.0480	1.3070	42.619	42.616
-1.2	0.9990	2.4800	43.599	43.598
-1.0	0.9705	3.5540	44.211	44.211
-0.8	0.9400	5.3040	44.907	44.909
-0.4	0.8703	14.790	46.683	46.690
0	0.7835	62.450	49.383	49.399
0.4	0.6845	356.30	53.481	53.511
0.8	0.5688	2788.0	60.719	60.763
1.2	0.4365	26 780	75.991	76.020

a. $\theta \equiv 5040/T$

b. [9].

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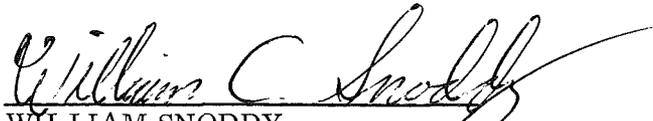
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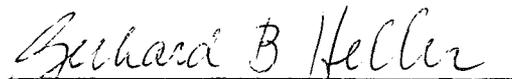
CALCULATIONS OF ASTROPHYSICAL
PARTITION FUNCTIONS

By M. J. Hagyard

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