

Senior astrophysics Lab 1: Line formation

Name:

Checkpoints due: Friday 23 March 2018

Contents

1	The Saha and Boltzmann equations	1
2	Exercise 1: The Saha-Boltzmann results for unobtainium	3
3	Exercise 2: Payne curves for unobtainium	8
4	Discussion	9

In this lab, you are going to investigate the way the Boltzmann and Saha equations influence the stellar spectra that we observe. In particular, we want to know why absorption lines of particular elements appear in the atmospheres of some stars and not other stars of different temperatures.

The Harvard spectral sequence, devised by Annie Jump Cannon, arranges stars based on their spectral characteristics. The final sequence is illustrated in Figure 1. It turns out to be an ordering in temperature, with the hottest stars (O and B) at the top and the coolest stars (K and M) at the bottom.

Inspection of this figure shows that the strengths of different lines varies smoothly between the classes. The calcium K line, on the left of the figure, is almost absent in B stars, then increases in strength to the F and G stars. The hydrogen lines, on the other hand, increase in strength from B to A stars, then decrease. We are going to show why the hydrogen lines are strongest in A stars.

1 The Saha and Boltzmann equations

Recall that the absorption lines we see in stellar atmospheres arise when electrons make transitions between two atomic energy levels. In order to understand what absorption lines we will see in spectra, we have to calculate how many atoms are in each state, for which we use the Saha and Boltzmann equations

1.1 The Boltzmann equation

The Boltzmann equation is used to calculate the distribution of electrons among the atomic orbitals in a single *ionisation state*, e.g. singly ionised helium He^+ (which astronomers

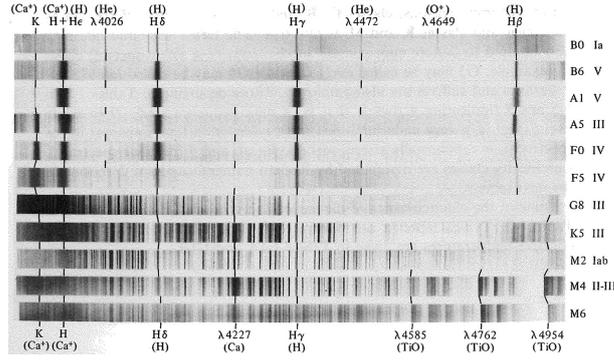


Figure 1: Representative stellar spectra illustrating the Harvard spectral sequence. The spectra are shown positively, with absorption lines dark on a bright background. From Novotny (1973).

denote He II), or neutral hydrogen (H I). The Boltzmann equation assumes the gas is in local thermodynamic equilibrium. Orbitals of higher energy are less likely to be occupied by electrons.

At temperature T , the populations n_1 and n_2 of any two energy levels are

$$\frac{n_2}{n_1} = \frac{g_2}{g_1} e^{-(E_2 - E_1)/kT} \quad (1)$$

where g_1 and g_2 are the statistical weights of the two levels.

In general, the number of electrons in any energy level s of an ionisation state i is given by

$$\frac{n_s}{N_i} = \frac{g_s}{Z_i} e^{-(E_s - E_1)/kT} \quad (2)$$

where N_i is the total number of particles in all energy levels in ionisation state i , $N_i = \sum_s n_s$, and Z_i is the partition function (see below).

1.2 The Saha equation

As the temperature increases, however, atoms will start becoming ionised. We use the Saha equation to calculate the relative number of atoms in different states of ionisation. The ratio of the number of atoms in ionisation state $(i + 1)$ to the number of atoms in state i is

$$\frac{N_{i+1}}{N_i} = \frac{2Z_{i+1}}{n_e Z_i} \left(\frac{2\pi m_e kT}{h^2} \right)^{3/2} e^{-\xi_i/kT} \quad (3)$$

where

- N_i is the number density of ions in ionisation state i
- n_e is the number density of electrons, which is related to the electron pressure via $P_e = n_e kT$
- m_e the electron mass
- ξ_i the ionisation energy from the ground state in ionisation state i
- Z_i and Z_{i+1} are the **partition functions** of ionisation states i and $i+1$: the weighted sum of the number of ways the atom can arrange its electrons with the same energy:

$$Z = \sum_{s=1}^{\infty} g_s e^{-(E_s - E_1)/kT} \quad (4)$$

For the following exercises, some Matlab code has been provided for you. Download it from eLearning (under “Computer lab 1”), or it is reproduced here. Hints as to how to start the problem are shown below as **MATLAB HINT**, if you’re having problems – but feel free to find your own, better, solution!

2 Exercise 1: The Saha-Boltzmann results for unobtainium

We are going to investigate a hypothetical iron-like element in conditions similar to a stellar atmosphere;¹ This element, which we will call **unobtainium** (Ub), has the following properties:

- ionisation energies $\xi_1 = 7$ eV for neutral Ub, $\xi_2 = 16$ eV for Ub^+ , $\xi_3 = 31$ eV for Ub^{2+} , and $\xi_4 = 51$ eV for Ub^{3+} .
- excitation energies that increase incrementally by 1 eV: $\xi_s = s-1$ eV in each ionisation state
- statistical weights $g_s = 1$ for all levels s .

Figure 2 shows the energy level diagram for the four ionisation states of Ub.

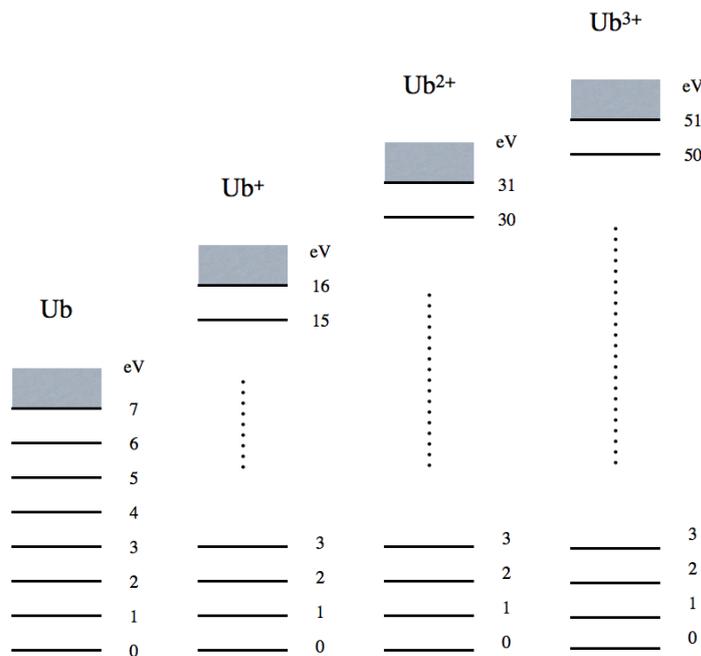


Figure 2: Energy level diagram for the element unobtainium (Ub), showing the neutral state (lefthand column, $i = 1$) and the first three ionization states ($i = 2-4$). In astronomical convention the spectra of neutral unobtainium Ub, ionised unobtainium Ub^+ and doubly ionised unobtainium Ub^{2+} are called Ub I, Ub II and Ub III respectively.

Your goal is to work out which ions will have significant transitions at which temperatures, which will mean evaluating the Saha and Boltzmann equations.

¹This exercise is based on a lab exercise written by Rob Rutten, from the University of Utrecht, www.staff.science.uu.nl/~rutte101/Exercises.html. He called his element “schadeenium”, after Dutch solar physicist Aert Schadee, but since that is unpronounceable to non-Dutch speakers, I have called it “unobtainium”.

Q1 First, you need to compute the partition function Z_i for each ionisation state of unobtainium. The file `partition_Ub.m` computes Z_i for each of the four ionisation states:

```
function z = partition_Ub(T)
    keV=8.61734e-5;           % Boltzmann's constant in eV/K
    chiion=[7,16,31,51];     % ionisation potentials for Ub

    z = [0,0,0,0];
    for i=1:4
        E = [1:1:chiion(i)]; % energy levels all 1 eV apart
        weight = exp(-(E-1)/(keV*T));
        z(i) = sum(weight);
    end % for i ...
    partition_Ub = z;
```

(Note that because our energy is in eV, we need to use Boltzmann's constant in eV/K, not J/K).

Fill in the following table for three different temperatures; the first has been done for you, as a check.

MATLAB HINT: Create a vector of the temperatures and calculate the partition function for each one:

```
T = [5000,10000,20000]; %create a vector of the temperatures
for t = 1:length(T) %for each temperature
    Z(:,t) = partition_Ub( T(t) );
end
```

Z_i	5000 K	10,000 K	20,000 K
Z_1	1.11		
Z_2	1.11		
Z_3	1.11		
Z_4	1.11		

Table 1: Partition function Z_i for the four ionisation states of Ub at different temperatures

Note that the partition functions are of order unity and barely sensitive to temperature.

Q2 Now you need to use equation 1 to compute the Boltzmann population for each energy level. The file `boltzmann_Ub.m` calculates the proportion of electrons in level s for ionisation state i , n_s/N_i for unobtainium.

```
function relnum = boltzmann_Ub(T,i,s)
    keV=8.61734e-5;           % Boltzmann's constant in eV/K

    z = [0,0,0,0];
    z=partition_Ub(T);
    relnum = 1/z(i) * exp (-(s-1)/(keV*T));
```

Use this function to fill in the following table, for neutral unobtainium (ionisation state 1).

MATLAB HINT: This time, you will need to create a vector of energy states S

```
S = [1,2,3,4,5,6,7,10,15]; %index the different energy levels in Ub
```

and then loop over each temperature T and each energy state S , and call `boltzmann_Ub` to calculate n_s/N_i .

```
for t = 1:length(T) %for each temp
    for s = 1:length(S) %for each energy state
        nsonNi(s,t) = ...
    end
end
```

n_s/N_1	5000 K	10,000 K	20,000 K
$s = 1$	0.90		
2	0.09		
3	0.01		
4	$O(-3)$		
5	$O(-4)$		
6	$O(-5)$		
7	$O(-6)$		
10	-		
15	-		

Table 2: Level population n_s/N_1 for unobtainium at different temperatures. The notation $O(-x)$ stands for order of magnitude 10^{-x} – too small to care about. (Note that levels 10 and 15 do not exist in the neutral atom)

Note the steep population decay with $E_s - E_1$, and that the decay is less steep for higher temperature.

Which energy level always has the largest population? Why?



Tutor's initials

Q3 Now you need to calculate the proportion of Ub in each ionisation state, N_i/N_{tot} . The simplest way to get this ratio is to set N_1 to some value (like 1), evaluate the four next ionisation state populations successively from equation 3, and divide them by their sum = N_{tot} in the same scale: examine the function `saha_Ub.m`.

```
function saha = saha_Ub(T,pe,ionstage)
% Compute Saha population fraction N_r/N for Unobtanium
% Inputs: temperature, electron pressure, ion stage
keV=8.61734e-5;           % Boltzmann's constant in eV/K
k=1.38065e-23;           % Boltzmann's constant in J/K
h=6.62607e-34;           % Planck's constant in Js
me=9.10938e-31;          % electron mass in kg

chiion=[7,16,31,51];     % ionisation potentials for Ub

ne = pe/(k*T);
z=partition_Ub(T);
z = [z 2];               % add estimated 5th value to get Z_4 too
sahaconst=(2.*pi*me*k*T/h^2)^1.5 * 2. / ne;
nion(1) = 1;
for i=1:4
    nion(i+1)=nion(i)*sahaconst*z(i+1)/z(i)*exp(-chiion(i)/(keV*T));
end % for i ...
ntotal = sum(nion);
nstagerel = nion ./ ntotal;
saha = nstagerel(ionstage);
```

Assume $P_e = 100$ Pa.

N_i/N_{tot}	ion	5000 K	10,000 K	20,000 K
i=1	Ub	0.91		
2	Ub ⁺	0.09		
3	Ub ²⁺	$O(-11)$		
4	Ub ³⁺	$O(-36)$		

Table 3: Population in each ionisation state N_i/N_{tot}

Note that there are only two ionisation stages significantly present per column. In other words, at a given temperature we will see lines of only two ionisation stages; the other lines vanish.

Q4 Finally, find the predicted strength of spectral lines from the neutral and ionised states of element Ub. Write a function `sahabolt_Ub.m(T,pe,i,s)` that evaluates N_s/N_{tot} for any level s as a function of temperature T and electron pressure P_e . You can find this by multiplying together your last two functions. Fill in the following table for the ground state of Ub, $s = 1$, assuming $P_e = 100$ Pa again.

N_1/N_{tot}	ion	5000 K	10,000 K	20,000 K
i=1	Ub	0.82		
2	Ub ⁺	0.08		
3	Ub ²⁺	$O(-11)$		
4	Ub ³⁺	$O(-37)$		

Table 4: Population in N_1/N_{tot}



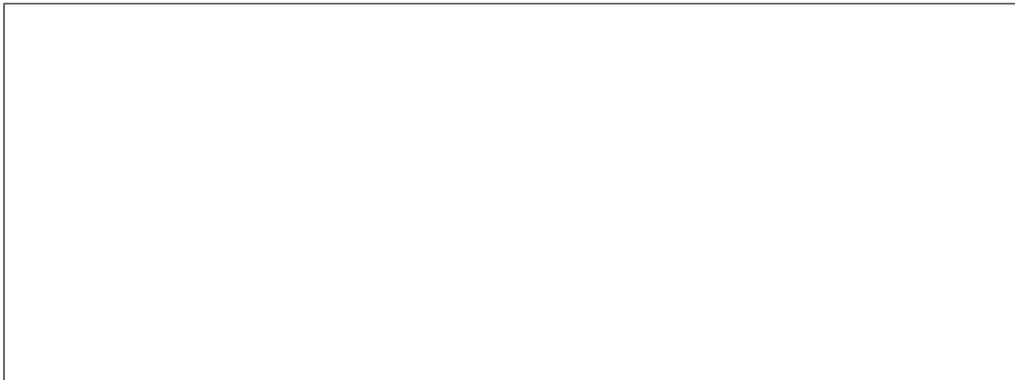
Tutor's initials

3 Exercise 2: Payne curves for unobtainium

Q1 Now for each ionisation state i , compute the ground-state population N_1/N_{tot} for a pressure $P_e = 100$ Pa as a function of temperature. Use temperatures ranging from 0 to 30,000 K. Plot all four ionisation states on the same graph with different line styles or colours.



What does this graph tell you about what you would see in the spectra of stars?



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4 Discussion

You have just repeated the work of Cecilia Payne at Harvard. In her 1925 thesis², she applied the newly derived Saha distribution for different ionisation states of an element to stellar spectra, and proved that the empirical Harvard classification represents primarily a temperature scale. The key graph in her thesis (published earlier in Payne 1924) is shown below in Fig. 3.

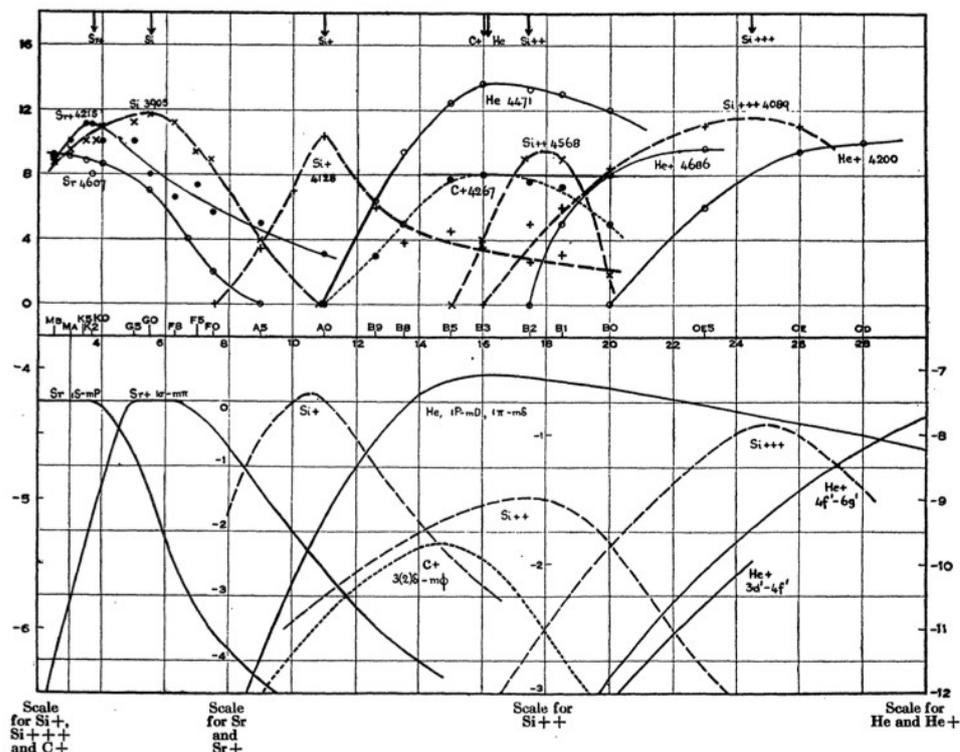


Figure 3: Strengths of selected lines along the spectral sequence. Upper panel shows observed line strengths; lower panel shows the Saha-Boltzmann predictions of the fractional concentration N_s/N_{tot} for the lower level of the lines indicated in the upper panel. From Payne (1924).

Her work showed that the great variation in stellar absorption lines was not due to differing chemical composition, but arose simply because of the different ionisation conditions in stars of different temperature. She correctly suggested that the proportion of heavy elements in stars was similar to that on Earth, but that hydrogen and helium are vastly more abundant (for hydrogen, by a factor of about one million). Her thesis thus established for the first time that hydrogen is the overwhelming constituent of the stars.

The Ub curves in your plot do indeed resemble Payne’s curves. In order to reproduce her lower panel in detail, you would have to evaluate the partition functions for the actual elements that she used and to enter the actual excitation energies of the lower levels of the lines that she used. More work, but in principle not different from what you have done for Ub. So, you have confirmed Payne’s conclusion that the Harvard classification of stellar spectra is primarily an ordering with temperature, controlled by Saha-Boltzmann population statistics.

²described by Otto Struve as “undoubtedly the most brilliant PhD thesis ever written in astronomy”.