ASTR 545 Fall 2018
Homework 5B (145 points)
ALWAYS SHOW YOUR WORK

Throughout this assignment, we adopt the notation n_{ijk}, n_{jk}, and n_k etc., where i is the excitation level, j is the ionization stage, and k is the species index. I have included two data files for your convenience. The first is the ionization potentials ("IonPotentials.txt") and the second is the partition functions ("PartFuncs.txt") of the relevant atoms and ions.

1. (20 pts) Ionization Fractions of Calcium. We will assume that there are three ionization stages for calcium, with number densities denoted $n_{1,20}$ for neutral, $n_{2,20}$ for singly ionized, and $n_{3,20}$ for doubly ionized, where the total calcium number density is $n_{20} = n_{1,20} + n_{2,20} + n_{3,20}$.

   (a) [4 pts] Starting with the definition of ionization faction for stage j, $f_{j,20} = n_{j,20}/n_{20}$, where $j = 1, 2, 3$, show that

$$f_{1,20} = \frac{1}{1 + Y_{1,20} + Y_{1,20}Y_{2,20}}\,, \quad f_{2,20} = f_{1,20}Y_{1,20}\,, \quad f_{3,20} = f_{2,20}Y_{2,20}\,, \tag{1}$$

   where $Y_{j,20} = n_{j+1,20}/n_{j,20}$.

The first ionization stage is determined via

$$f_{1,20} = \frac{n_{1,20}}{n_{20}} = \frac{n_{1,20}}{n_{1,20} + n_{2,20} + n_{3,20}}$$

$$f_{1,20} = \frac{n_{1,20}/n_{1,20}}{1 + n_{2,20}/n_{1,20} + n_{3,20}/n_{1,20}}$$

$$f_{1,20} = \frac{1}{1 + n_{2,20}/n_{1,20} + (n_{3,20}/n_{2,20})(n_{2,20}/n_{1,20})}$$

$$f_{1,20} = \frac{1}{1 + Y_{1,20} + Y_{1,20}Y_{2,20}}$$

The second ionization stage is determined via

$$f_{2,20} = \frac{n_{2,20}}{n_{20}} = \frac{n_{2,20}}{n_{1,20} + n_{2,20} + n_{3,20}}$$

$$f_{2,20} = \frac{n_{2,20}/n_{1,20}}{1 + n_{2,20}/n_{1,20} + (n_{3,20}/n_{2,20})(n_{2,20}/n_{1,20})}$$

$$f_{2,20} = \frac{Y_{1,20}}{1 + Y_{1,20} + Y_{1,20}Y_{2,20}}$$

$$f_{2,20} = f_{1,20}Y_{1,20}$$

The third ionization follows by obtaining $(n_{3,20}/n_{2,20})(n_{2,20}/n_{1,20}) = Y_{1,20}Y_{2,20}$ in the numerator with the identical denominator as for $f_{1,20}$ and $f_{2,20}$. It follows that

$$f_{2,20} = \frac{Y_{1,20}Y_{2,20}}{1 + Y_{1,20} + Y_{1,20}Y_{2,20}} = f_{2,20}Y_{2,20}$$

(b) [10 pts] Invoking $Y_{j,20} = n_{j+1,20}/n_{j,20} = n_e^{-1}\Phi_{j,20}(T)$, compute the calcium ionization fractions in the atmosphere of a G3 Ia star with $T = 6000$ K and $n_e = 8 \times 10^{11}$ cm^{-3}.

$f_{1,20} = 2.592 \times 10^{-5}$
$f_{2,20} = 8.894 \times 10^{-1}$
$f_{3,20} = 1.106 \times 10^{-1}$

(c) [4 pts] Recompute the calcium ionization fractions in the atmosphere of a G3 V star with $T = 6000$ K and $n_e = 2 \times 10^{13}$ cm^{-3}.

$f_{1,20} = 7.245 \times 10^{-4}$
$f_{2,20} = 9.943 \times 10^{-1}$
$f_{3,20} = 4.946 \times 10^{-3}$

(d) [2 pts] Assuming these stars have identical metallicities and abundance patterns, which star, the G3 V or the G3 Ia, will have the stronger Ca II H&K lines in its spectrum? Based on physical principles, explain why this occurs.

The ionizationf fraction of Ca II in the G3 V star is higher than it is in the G3 Ia star. There for the number denisty of Ca II is larger in the G3 V star than in the G3 Ia star. Since the line opacity scales with the number density, $\chi_\lambda = n_{2,20}\sigma(\lambda)$, and the cross section is the same for the thermal conditions of both stars, the optical depth, $\tau_\lambda = \int_0^L \chi_\lambda ds$, will be higher in the G3 V star (this also assumes the the pathlength over which the absorption is occuring are the same (in addition to the temperature, metallicities, and adundances). Thus, the Ca II H&K absorption lines willbe larger in the G3 V star.

2. (10 pts) Excitation and Ionization– the "Balmer Hydrogen".

(a) [4 pts] Starting with the Boltzmann excitation equation for n_{211}/n_{11}, and the Saha ionization equation for n_{21}/n_{11}, combine them to derive the expression for the quantity n_{211}/n_1, i.e., the number density of neutral hydrogen atoms in the $n = 2$ excitation state relative to the number density of all hydrogen.

$$\frac{n_{211}}{n_1} = \frac{n_{211}}{n_{11}}\frac{n_{11}}{n_1} \quad \text{where} \quad \frac{n_{211}}{n_{11}} = \frac{g_{211}}{U_{11}(T)} \exp\{-\chi_{211}/kT\}$$

and

$$\frac{n_{11}}{n_1} = f_{11} = \frac{1}{1+Y_{11}} = \frac{1}{1+n_e^{-1}\Phi_{11}(T)}$$

yielding

$$\frac{n_{211}}{n_1} = \frac{n_{211}}{n_{11}}\frac{n_{11}}{n_1} = f_{11}\frac{g_{211}}{U_{11}(T)} \exp\{-\chi_{211}/kT\} = \frac{g_{211}}{U_{11}(T)}\frac{\exp\{-\chi_{211}/kT\}}{1+n_e^{-1}\Phi_{11}(T)}$$

where $\Phi_{11}(T) = C_\Phi T^{3/2}\,[U_{21}(T)/U_{11}(T)]\exp\{-R_{11}/kT\}$ where $C_\Phi = 4.8 \times 10^{15}$ cm^{-3} K$^{-3/2}$, with $\chi_{211} = R_{11}(1 - 1/2^2) = 10.199$ eV, and $R_{11} = 13.598$ eV.

(b) [6 pts] Using your expression, for the gas conditions you computed for Problem 2 in Homework 5A, compute n_{211}/n_1. Now compute n_{211}. [I recommend adding this calculation to your existing code]

Here are some intermediate results: $\Phi_{11} = 6.774 \times 10^{14}$ cm^{-3} and $Y_{11} = 10.71$. The ratio is $n_{211}/n_1 = 2.476 \times 10^{-6}$, giving $n_{211} = 1.620 \times 10^8$ cm^{-3}.

3. (50 pts) Equilibrium Gas Physics. Consider a gas structure in thermal equilibrium with $T = 6000$ K and $P_g = 100$ dynes cm^{-2} comprising hydrogen, helium, and one metal, calcium, with mass fractions $X = 0.71$, $Y = 0.27$, and $Z = 0.02$. Assume all ionization states for H and He and that Ca can be ionized twice (Ca^0, Ca^+, Ca^{+2}). Compute the equilibrium conditions of the gas using particle-charge conservation,

$$n_e = (n - n_e) \sum_k \alpha_k \sum_{j=1}^{J_k} (j-1) f_{jk}(n_e, T) \tag{2}$$

In solving Eq. 2, apply a tolerance of at least $n_e^+ - n_e^- = 10^{-5}$, where n_e^+ and n_e^- are the values that bracket the root, n_e. I have provided the solutions to this problem so you can ensure you are obtaining the correct equilibrium solution for all ionization stages of all species. Please present your solutions in the identical format.

(a) [15 pts] Table 1. For the given T and P_g, report the abundance fractions, α_k and the densities $n_{\rm N}$, n_e, and n.

See the separate file: 'HW5B-P3-Solutions.txt'

(b) [15 pts] Table 2. Report the equilibrium values $n_{\rm N}$, n_e, $\mu_{\rm N}$, μ_e, μ, $\rho_{\rm N}$, ρ_e, ρ, P_e, and P_e/P_g.

See the separate file: 'HW5B-P3-Solutions.txt'

(c) [15 pts] Table 3. Report the equilibrium values n_k, n_{jk}, f_{jk}, $\Phi_{jk}(T)$, $\log U_{jk}(T)$ and fraction of electrons donated for ion $j, k,$, i.e., $f(n_e, j, k) = (j-1)\, n_{jk}/n_e$.

See the separate file: 'HW5B-P3-Solutions.txt'

(d) [5 pts] From Table 3, identify and rank which ionization stages of which species are the top three donors of free electrons to the gas. What do these data tell you about the role of metals in gas where hydrogen and helium are not highly ionized?

See the separate file: 'HW5B-P3-Solutions.txt'

4. (65 pts) Equilibrium Gas Physics as a Function of Temperature. Expand your code to compute the equilibrium conditions of this gas structure over the range $1500 \leq T \leq 25{,}000$ K. I provided solutions to this problem in the form of several plots. Reproduce the plots and hand in your versions. Answer the below questions.

(a) [20 pts] Plot 1: Densities, Molecular Weights, and Pressure
Panel 1a: $\log n_e$, $\log n_N$, and $\log n$
Panel 1b: $\log \rho_e$,$\log \rho_N$, and $\log \rho$
Panel 1c: $\log \mu_e$,$\log \mu_N$, and $\log \mu$
Panel 1d: $P_e/P_{\rm g}$.

See the separate file: 'Plot1.pdf'

(b) [20 pts] Plot 2: Ionization Fractions and Atom/Ion Densities
Panel 2a: f_{jk} for hydrogen; Panel 2b: $n_k j$ and n_{jk} for hydrogen
Panel 2c: f_{jk} for helium; Panel 2d: $n_k j$ and n_{jk} for helium
Panel 2e: f_{jk} for calcium; Panel 2f: $n_k j$ and n_{jk} for calcium.

See the separate file: 'Plot2.pdf'

(c) [10 pts] Plot 3: Fraction Contributions to Free Electrons
Plot 3: $\log f(n_e)$, where $f(n_e) = (j-1)\, n_{jk}/n_e$, for all jk.

See the separate file: 'Plot3.pdf'

(d) [3 pts] Examining Plot 1, explain why n and ρ decrease with increasing T, and why they have the slopes they do.

Since the total pressure of the gas is help constant, the number density scales as $n \propto P_g/kT$. Thus, as the temperature is increased, the number density (and mass density) decrease. On a log-log plot, the slope is $\partial \log n/\partial \log T = -1$. The same argument holds for the mass density, ρ, in that $\partial \log \rho/\partial \log T = -1$. (I know that Plot 1, as shown, is linear in T, but the description above is correct in principle).

(e) [4 pts] On Plot 1, what is the physical reason for the rise, turnover, and rise again of n_e and ρ_e across the temperature range 2000-7000 K? (HINT: examine the behavior of Plot 2).

For $T \leq 2000$ K there are virtually a vanishingly small number of electrons in the gas, as no atoms are being significantly ionized yet. As the temperature rises to about 3500 K, Ca I becomes fully ionized, so from 2500 to 3500 K we see an increase in n_e, and calcium is dominated by the Ca II stage. Thus, the rise of n_e in this temperature range is due to the ionization of Ca I to Ca II. The temperature must rise to 5000 K in order for H I to start ionizing (note that this is when Ca II starts ionizing into Ca III as well). Since H dominates the number density, the rapid rise in n_e from 5000 to 10,000 K is due to the ionization of H I to H II (the Ca III has negligible contribution). The reason for the apparent "decrease" in n_e in the range 3500 to 5000 is an artifact of the fact that we enforce a constant gas pressure for the gas; as temperature rises from 3500 to 5000 K, the overall density thus decreases per the behavior described in part (d).

(f) [3 pts] From Plot 3 report which ionization species is the major electron donor in each temperature range as a function of temperature.

For $T \leq 5000$ K, Ca I dominates. For $T \geq 5000$ K, H I dominates. For $T \geq 15,000$ K, He I contributes roughly 10%.

(g) [5 pts] Going back to Plot 1, note that $P_e/P_{\rm g}$ rises to 0.5, levels off, and then rises slightly above 0.5. Explain physically why this is happening (i.e., why $\simeq 0.5$, and then slightly above 0.5?).

> I understand that this has been a problem result for most of you in that you do not get the bump above $P_e/P_g = 0.5$ at $T \geq 15,000$ K. None the less, I will explain my result. In a pure hydrogen gas, when the hydrogen is fully ionized we have $n_e = n_{\rm H}$, so that $P_e/P_g = n_e/(n_e + n_{\rm H}) = 1/2$. In our gas, since hydrogen totally dominates the gas by number density, when the hydrogen is fully ionized we should roughly obtain the same ratio, which occurs when for $T \geq 10,000$ K (note, however, that my curve does not reach 0.5 until helium begins to contribute a very small additional fraction to the electron pool). Then above $T \geq 15,000$ K ionization of He I is complete and we have a roughly 10% increment in the ratio P_e/P_g.

5. (15 pts EXTRA CREDIT) Hydrogen Excitation. Add hydrogen excitation to your code and plot the ratios n_{111}/n_1, n_{211}/n_1, and n_{311}/n_1 as a function of T for the equilibrium physics of your gas in Problem 4.

YOUR CODES Hand in hard copies of your codes in class. Upload your results to Canvas.