Saha Equation of State

Math Document

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1 Saha Equation

The general Saha equation is given by

$$\frac{n_i^{r+1}}{n_i^r} = \left(\frac{2\pi m_e k}{h^2}\right)^{\frac{3}{2}} T^{\frac{3}{2}} \frac{2B_i^{r+1} exp\left(\frac{-\chi_i^r}{kT}\right)}{B_i^r N_e} \tag{1}$$

where for element i and ionization r. For ease of expression, we will take

$$C_i = \left(\frac{2\pi m_e k}{h^2}\right)^{\frac{3}{2}} \frac{2B_i^{r+1}}{B_i^r} \tag{2}$$

So the Saha equation is re-expressed by

$$\frac{n_i^{r+1}}{n_i^r} = C_i T^{\frac{3}{2}} exp\left(\frac{-\chi_i^r}{kT}\right) \frac{1}{N_e} \tag{3}$$

This is the form we will manipulate throughout this document.

1.1 Iterative Method

Initially, the iterative method using the Saha equation was as follows:

1. Choose a temperature T and a density ρ
2. Guess an initial electron density N_e
3. Solve $\frac{n_i^{r+1}}{n_i^r}$ for all ratios applicable to element i. Hydrogen, for example, only has $\frac{n_H^1}{n_H^0}$
4. Use the ratios to solve the ionization fraction, given by

$$y_i^r = \frac{n_i^r}{\sum_{s=0}^{z(i)} n_i^s} \tag{4}$$

5. Use y_i^r to solve for the average number of free electrons contributed by element i using

$$\nu_e(i) = \sum_{s=0}^{z(i)} s y_i^s \tag{5}$$

6. Recompute the electron density as

$$N_{e1} = \rho N_o \sum_i \frac{x_i}{A_i} \nu_e(i) \tag{6}$$

   where N_o is Avogadro's number, x_i is the grams of element i per grams grams of mixuture, and A_i is the standard atomic weight of element i.

There steps are repeated until N_e and N_{e1} are within some tolerance.

1.1.1 Computing the ionization fraction

We must manipulate equation 4 because once we compute the Saha equation, we only have the ratios $\frac{n_i^{r+1}}{n_i^r}$. We will give examples of the new ionization fraction equations which is a bit more straightforward than just an equation. Also, we never need to compute the value y_i^0 because it contributes zero electrons to the recalculation of the electron density.

Hydrogen For hydrogen, we only have the ratio $\frac{n^1}{n^0}$, where we have dropped the subscript denoting the element to reduce clutter. The only ionization fraction we need to compute is then given by

$$y^1 = \frac{n^1}{n^0 + n^1} = \frac{1}{\frac{n^0}{n^1} + 1}$$

$$y^1 = \frac{1}{\frac{1}{\frac{n^1}{n^0}} + 1} \tag{7}$$

Helium For helium, we have the ratios $\frac{n^1}{n^0}$ and $\frac{n^2}{n^1}$ and we have two ionization fraction we must compute. The first is given by

$$y^1 = \frac{n^1}{n^0 + n^1 + n^2} = \frac{1}{\frac{n^0}{n^1} + 1 + \frac{n^2}{n^1}}$$

$$y^1 = \frac{1}{\frac{1}{\frac{n^1}{n^0}} + 1 + \frac{n^2}{n^1}} \tag{8}$$

and the second is given by

$$y^2 = \frac{n^2}{n^0 + n^1 + n^2} = \frac{1}{\frac{n^0}{n^2} + \frac{n^1}{n^2} + 1} = \frac{1}{\frac{1}{\frac{n^2}{n^0}} + \frac{1}{\frac{n^2}{n^1}} + 1}$$

$$y^2 = \frac{1}{\frac{1}{\frac{n^1}{n^0}\frac{n^2}{n^1}} + \frac{1}{\frac{n^2}{n^1}} + 1} \tag{9}$$

Carbon TODO

1.1.2 Using the computed electron density

2 Pressure

The general expression for pressure is given by

$$P = nkT \tag{10}$$

where we have $n = n_i + N_e$ which includes the number of particles of a given element i and the number of free electrons. Therefore

$$P = (n_i + N_e)kT \tag{11}$$

In the following sections, we will examine how the equation of pressure changes when considering various elements.

3 Internal Energy

4 Mixture of Pure Hydrogen

4.1 The Saha Equation

The Saha equation for hydrogen is given by

$$\frac{n_H^1}{n_H^0} = C_H T^{\frac{3}{2}} exp\left(\frac{-\chi_H^0}{kT}\right)\frac{1}{N_e} \tag{12}$$

where

$$C_H = \left(\frac{2\pi m_e k}{h^2}\right)^{\frac{3}{2}} \frac{2B_H^1}{B_H^0}$$

4.2 Pressure

The pressure of an ionized mixture of pure hydrogen is given by

$$P = (n_H + N_e)kT \tag{13}$$

and we can express the number of hydrogen atoms as

$$n_H = \rho N_o \frac{x_H}{A_H} \tag{14}$$

where $A_H = 1.00794$ and $x_H = 1$.

4.2.1 Manipulation of the Saha equation

Solving for temperature from pressure

$$P = (n_H + N_e)kT$$

$$T = \frac{P}{(n_H + N_e)k} \tag{15}$$

Now use the temperature in equation 15 in

$$\frac{n_H^1}{n_H^0} = \left(\frac{2\pi m_e k}{h^2}\right)^{\frac{3}{2}} \frac{2B_H^1}{B_H^0} T^{\frac{3}{2}} exp\left(\frac{-\chi_H^0}{kT}\right)\frac{1}{N_e} \tag{16}$$

We will now define a function $g(N_e)$ by substituting T into equation 16

$$\frac{n_H^1}{n_H^0} = g(N_e) = C_H \left(\frac{P}{(n_H + N_e)k}\right)^{\frac{3}{2}} exp\left(\frac{-\chi_H^0}{k_{eV}\left(\frac{P}{(n_H+N_e)k}\right)}\right)\frac{1}{N_e} \tag{17}$$

Using $g(N_e)$, we can express the ionization fraction as

$$y_H^1 = \frac{1}{\frac{1}{g(N_e)} + 1} \tag{18}$$

We then have

$$\nu_e(H) = 1 * y_H^1 = y_H^1 \tag{19}$$

Therefore, we want to solve

$$N_e = n_H * \nu_e(H) = n_H * y_H^1 = n_H * \frac{1}{\frac{1}{g(N_e)} + 1} \tag{20}$$

$$N_e = n_H * \frac{1}{\frac{1}{C_H\left(\frac{P}{(n_H+N_e)k}\right)^{\frac{3}{2}} exp\left(\frac{-\chi_H^0}{k_{eV}\left(\frac{P}{(n_H+N_e)k}\right)}\right)\frac{1}{N_e}} + 1} \tag{21}$$

It is clear that equation 21 is nonlinear, however we should be able to use root finding numerical methods to solve it... should. We can use $G(N_e)$ for this.

$$G(N_e) = n_H * \frac{1}{\frac{1}{C_H\left(\frac{P}{(n_H+N_e)k}\right)^{\frac{3}{2}} exp\left(\frac{-\chi_H^0}{k_{eV}\left(\frac{P}{(n_H+N_e)k}\right)}\right)\frac{1}{N_e}} + 1} - N_e = 0 \tag{22}$$

Solving for N_e from pressure

$$P = (n_H + N_e)kT \rightarrow \frac{P}{kT} = n_H + N_e$$

$$N_e = \frac{P}{kT} - n_H \tag{23}$$

Also

$$kTN_e = P - n_H kT \tag{24}$$

4.3 Internal Energy

4.3.1 Manipulation of the Saha equation

Solving for temperature from internal energy

Solving for N_e from internal energy