Webnucleo Technical Report: Low-Temperature Nuclear Statistical Equilibria

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This technical report discusses nuclear statistical equilibria at low temperature and calculations with libnuceq.

1 Introduction

libnuceq is a library of C codes for computing nuclear statistical equilibria relevant to nucleosynthesis. Libnuceq codes can compute most equilibria fairly robustly, though they can run into difficulty at very low temperatures. Of course, equilibrium is difficult to attain at low temperature; nevertheless, it is useful to consider these solutions.

2 Free Energy Minimization

At fixed temperature and volume (or mass density), equilibrium occurs at a minimum in the Helmholtz free energy per nucleon f. This quantity is given by

$$f = \varepsilon - Ts \tag{1}$$

where ε is the energy per nucleon, T is the temperature, and s is the entropy per nucleon. The energy per nucleon (assuming non-relativistic, non-degenerate particles) is

$$\varepsilon = \sum_i \left(\frac{3}{2}kT + m_i c^2 \right) Y_i, \tag{2}$$

where $m_i c^2$ is the rest mass energy of species i and Y_i is the abundance per nucleon of species i. The sum in Eq. (2) runs over all species, including electrons. Because of charge neutrality in our assumed fully ionized plasma,

$$\sum_{i \in nuc} Z_i Y_i = Y_e \tag{3}$$

where Y_e is the net electron number per nucleon, and the sum runs only over nuclear species. From Eq. (3), we may write

$$\varepsilon = \sum_{i \in nuc} \left(m_i c^2 + Z_i m_e c^2 \right) Y_i + \frac{3}{2}kT \sum_{i \in nuc} (1 + Z_i) Y_i, \tag{4}$$

where $m_e c^2$ is the rest mass energy of the electron. If we neglect the binding energy of electrons in an atom relative to the nuclear rest mass energy, Eq. (4) becomes

$$\varepsilon = \sum_{i \in nuc} m_i^{atomic} c^2 Y_i + \frac{3}{2} kT \sum_{i \in nuc} Y_i, \tag{5}$$

where $m_i^{atomic} c^2$ denotes the *atomic* rest mass energy of species i.

For classical, non-degenerate, non-interacting particles, the entropy per nucleon for species i is given by

$$s_i = \frac{5}{2} Y_i - Y_i \ln\left(\frac{Y_i}{Y_{Qi}}\right) \tag{6}$$

where the quantum abundance Y_{Qi} is

$$Y_{Qi} = \frac{G_i}{\rho N_A} \left(\frac{m_i kT}{2\pi\hbar^2}\right)^{3/2}. \tag{7}$$

From this, we may find

$$s = \sum_{i \in nuc} \frac{5}{2} (1 + Z_i) Y_i - k \sum_{i \in nuc} Y_i \ln\left(\frac{Y_i}{Y_{Qi}}\right) + kT \ln\left(\frac{Y_i}{Y_{Qe}}\right). \tag{8}$$

With Eqs. (5) and (8), Eq. (1) becomes

$$f = \sum_{i \in nuc} m_i^{atomic} c^2 Y_i - kT \sum_{i \in nuc} (1 + Z_i) Y_i + kT \sum_{i \in nuc} Y_i \ln\left(\frac{Y_i}{Y_{Qi}}\right) + kT Y_e \ln\left(\frac{Y_e}{Y_{Qe}}\right). \tag{9}$$

As $kT \to 0$, this becomes

$$f = \sum_{i \in nuc} m_i^{atomic} c^2 Y_i. \tag{10}$$

This result shows that, at low temperature, the system will tend to minimize the atomic mass per nucleon.

3 Two-Species Limit

At low temperatures, nuclear equilibria, if they can be attained, are dominated by one or two species. We consider a two species equilibrium. The conditions on a nuclear statistical equilibrium are then 1) mass conservation and 2) charge neutrality. Mass conservation requires

$$A_1 Y_1 + A_2 Y_2 = 1, \tag{11}$$

where A_1 and A_2 are the mass number of species 1 and 2, respectively, while Y_1 and Y_2 are their abundances per nucleon. Charge neutrality requires

$$Z_1 Y_1 + Z_2 Y_2 = Y_e, \tag{12}$$

where Z_1 and Z_2 are the atomic numbers of species 1 and 2. Solution of Eqs. (11) and (12) yield

$$Y_1 = \frac{1}{A_1} \left(\frac{Y_e^{(2)} - Y_e}{Y_e^{(2)} - Y_e^{(1)}}\right) \tag{13}$$

and

$$Y_2 = \frac{1}{A_2}\left(\frac{Y_e - Y_e^{(1)}}{Y_e^{(2)} - Y_e^{(1)}}\right). \tag{14}$$

In these equations,

$$Y_e^{(i)} = \frac{Z_i}{A_i}. \tag{15}$$

The free energy is then

$$f = m_1 c^2 Y_1 + m_2 c^2 Y_2 \tag{16}$$

Equilibrium occurs for the combination of two species that minimizes f for the given Y_e. If Y_e of the system is equal to the Z/A ratio of one of the two species, call it species 1, then $Y_1 = 1/A_1$ and $Y_2 = 0$, and a single species will dominate the equilibrium. The free energy per nucleon then becomes

$$f = \frac{m_1 c^2}{A_1}. \tag{17}$$

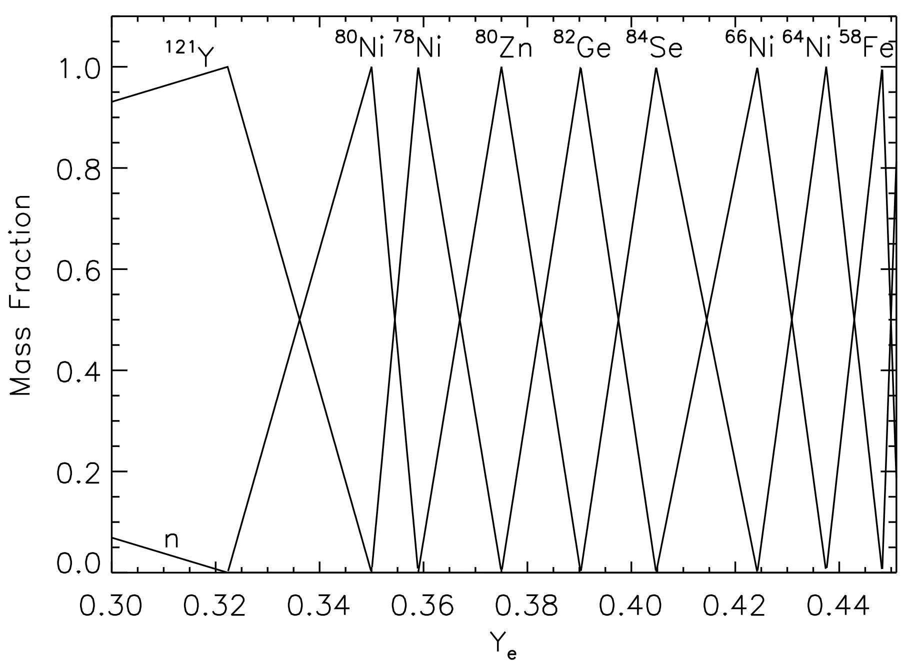

Figure 1: Mass fractions in a two-species, low temperature nuclear statistical equilibrium.

Figures 1 and 2 show the mass fractions that satisfy Eq. (16) for the mass file that comes with the libnuceq 0.1 distribution. At $Y_e = 0$, the system consists of only free

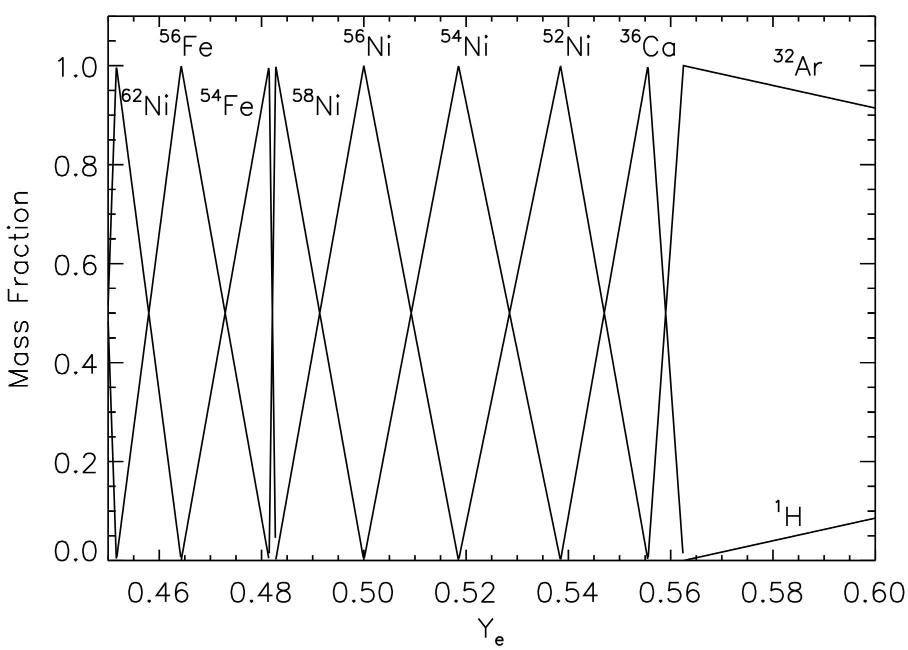

Figure 2: Mass fractions in a two-species, low temperature nuclear statistical equilibrium.

neutrons. As Y_e increases, the system becomes a mix of free neutrons and ^{121}Y. As Y_e increases further, the nuclei are able to lock up all the neutrons, and the system is dominated by a mix of various species (mostly in the iron group). At certain values of Y_e, the abundances are dominated by a single species with a Z/A ratio equal to the Y_e value. As Y_e increases to values greater than 0.56, the nuclei are not proton-rich enough to lock up all the protons, and the system becomes a mix of ^{1}H and ^{32}Ar. ^{32}Ar is the winner for very proton-rich nuclear statistical equilibria because, although it does not have a particularly large binding energy per nucleon, it is a particularly proton-rich species and can have a large abundance in proton-rich environments. Because it is bound, locking protons up into it reduces the overall nuclear mass per nucleon in the system, thereby reducing the free energy. At $Y_e = 1$, the system, of course, consists only of free protons.

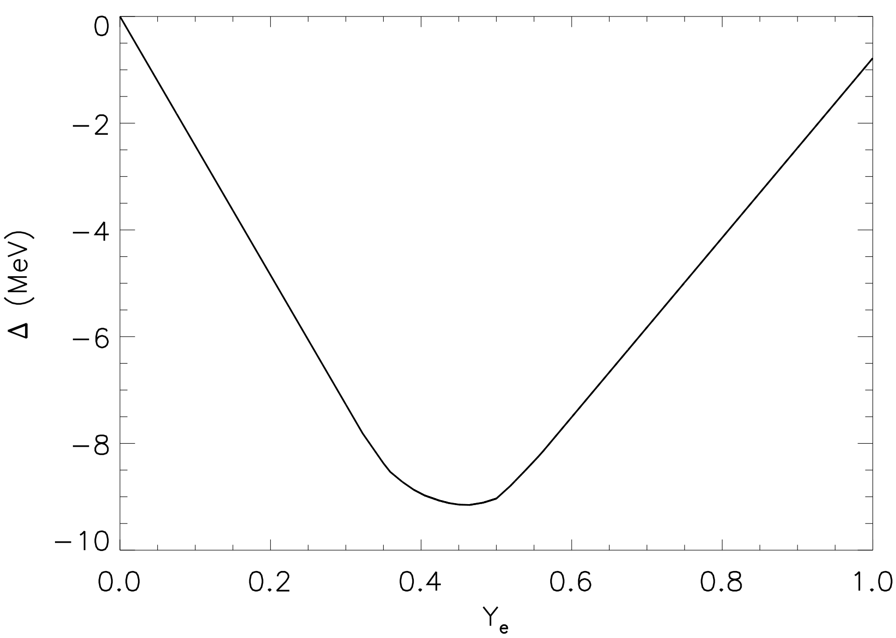

Figure 3: Atomic rest mass per nucleon relative to the neutron rest mass in a two-species low-temperature nuclear statistical equilibrium.

Figure 3 shows the atomic mass per nucleon relative to the neutron mass a function of Y_e. Figure 4 shows the same curve but on a more restricted range in Y_e. The sudden breaks in the slope of the curve in Figure 4 are real and are due to the sudden compositional changes evident in Figures 1 and 2. The minimum atomic mass per nucleon occurs at the Y_e corresponding to ^{56}Fe. Thus, the low-temperature system considered here would tend to evolve by weak interactions until it consisted entirely of electrons and ^{56}Fe. This is somewhat surprising, given that ^{56}Fe is not the nuclear species with the largest nuclear binding per nucleon–^{62}Ni is. The reason ^{56}Fe dominates is due to

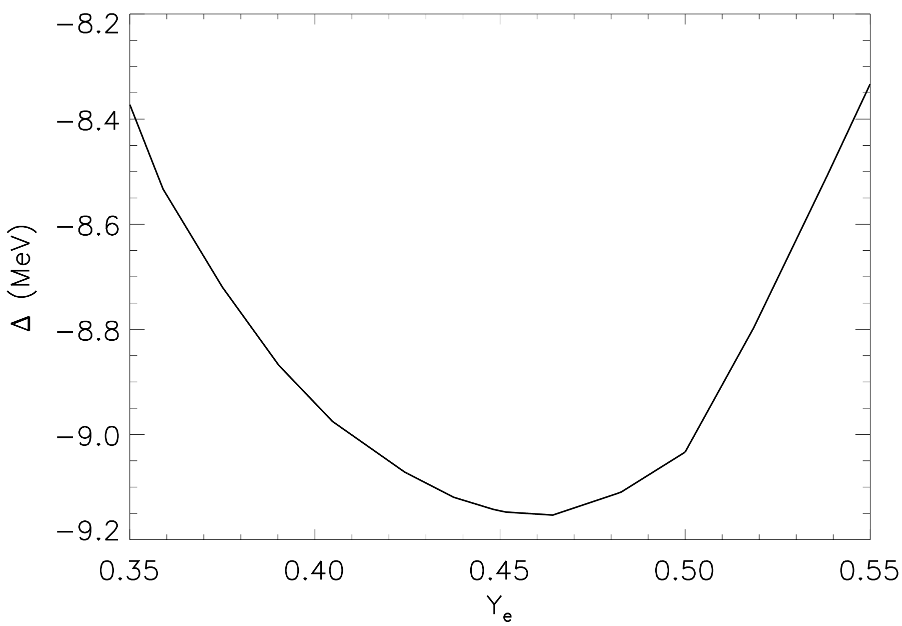

Figure 4: Atomic rest mass per nucleon relative to the neutron rest mass in a two-species low-temperature nuclear statistical equilibrium.

the fact that protons are less massive than neutrons, and the lower mass from the larger number of protons in the system dominated by ^{56}Fe more than compensates the tighter binding in the system dominated by ^{62}Ni.

4 Low Temperature Calculations with libnuceq

At low temperatures, libnuceq codes will calculate the correct nuclear statistical equilibrium, as determined by the above considerations. The difficulty will be that the accuracy of the abundances will not be good due to the extremely large absolute values of the neutron and proton chemical potentials. Recall that the abundance of species i in the equilibrium depends on the exponential of the quantity $Z_i \frac{\mu_p}{kT} + (A_i - Z_i) \frac{\mu_n}{kT}$. Numerical inaccuracies in the chemical potentials then propagate into the abundances.

Another problem occurs for low temperature calculations of weak nuclear statistical equilibrium. At low temperatures, the electron chemical potential can become extremely large during the root-finding iterations and the default calculation of the electron number density fails.

The above problems occur for extremely low temperatures (tens of Kelvins or less), which are not generally relevant to nuclear statistical equilibria of physical interest. At such low temperatures, one must consider that the system may not be a plasma and the classical expressions for nuclei are not relevant (the nuclei may become boson condensates!). Should the user be interested is very low temperature equilibria, he or she could extend the considerations in §3. libnuceq-based codes should be able to handle most other cases.