Unit 4

Distribution functions

In Unit 6 we will start to derive equations of state of stellar matter. To do so from first principles, we need to know how, in general, particles are distributed as a function of momentum (or energy). This requires some basic statistical mechanics.

Statistical mechanics deals with the occupation of energy states when a system is excited. The fundamental assumption of statistical mechanics is that, in thermal equilibium, every distinct state with the same total energy is occupied with equal probability. Temperature is simply a measure of the total energy of a system in thermal equilibium. The only change from classical statistical mechanics to quantum mechanics has to do with how we count distinct states, which depends on whether the particles involved are distinguishable, identical fermions, or identical bosons.

4.1 An example

- Consider 3 non-interacting particles of equal mass in some potential.
- The total energy of the system is 243 (with some arbitrary energy units). This means that the particles occupy some energy levels n_i such that, using a simple and arbitrary energy rule, we have

$$E_{\text{total}} = \sum_{i=1}^{\infty} n_i i^2 = 243. \tag{4.1}$$

  A one-dimensional square well, for example, has a dispersion relation like this one. There would be prefactors before the summation symbol to give the right units of energy; for simplicity, ignore such terms.

- Consider distinguishable (classical) particles. There are 13 unique ways of distributing 3 particles into various energy levels to get a total energy of 243.
  - We can have all 3 particles in the 9th state: $n_9 = 3$. There is only 1 way of doing this.
  - $n_1 = 1,\ n_{11} = 2$. (3 ways)
  - $n_3 = 2,\ n_{15} = 1$. (3 ways)
  - $n_5 = n_7 = n_{13} = 1$. (6 ways)
- Quantum statistics says, for large N, that all states with the same N and same E_{total} are equally likely.
- Therefore, in thermal equilibrium, the most probable configuration is the one that can be achieved in the largest number of ways. The last state is this case. We'll come back to this.
- Now consider fermions, which are indistinguishable, and cannot occupy the same state.

- There is only one possibility here: $n_5 = n_7 = n_{13} = 1$.
- Finally, consider bosons, which are indistinguishable. There are 3 distinct states:
  - $n_9 = 3$. (1 way)
  - $n_3 = 2,\ n_{15} = 1$. (1 way)
  - $n_5 = n_7 = n_{13} = 1$. (1 way)

4.2 Partition function

- Again consider N particles with the same masses. There are energy states E_i with degeneracies g_i (distinct states with same energy E_i). We distribute the N particles such that there are N_1 particles with energy E_1, N_2 particles with energy E_2, etc. We want to know how many different ways we can do this?
- We now define $Q(n_1, n_2, n_3, \ldots)$ to be the number of microscopically distinguishable arrangements that lead to the same macroscopic distribution.
- It is sometimes known as a partition function, or probability distribution function, or canonical ensemble, etc.
- Clearly, Q depends strongly on the type of particle we are considering, as the 3 cases below show (without derivation).

4.2.1 Distinguishable particles

In this case,

$$Q = N! \prod_{i=1}^{\infty} \frac{g_i^{n_i}}{n_i!}$$

To prove this, we go back to the previous illustration:

$$Q(n_9 = 3) = 3! \left(\frac{1^3}{3!} \right) = 1. \tag{4.2}$$

$$Q(n_3 = 2, n_{15} = 1) = 3! \left(\frac{1^2}{2!} \right) \left(\frac{1^1}{1!} \right) = 3. \tag{4.3}$$

$$Q(n_5 = 1, n_7 = 1, n_{13} = 1) = 3! \left(\frac{1^1}{1!} \right) \left(\frac{1^1}{1!} \right) \left(\frac{1^1}{1!} \right) = 6. \tag{4.4}$$

This confirms our earlier counting.

4.2.2 Identical fermions

In this case,

$$Q = \prod_{i=1}^{\infty} \frac{g_i!}{n_i!\,(g_i - n_i)!}.$$

So,

$$Q(n_5 = 1, n_7 = 1, n_{13} = 1) = \left(\frac{1!}{1!0!} \right) \left(\frac{1!}{1!0!} \right) \left(\frac{1!}{1!0!} \right) = 1. \tag{4.5}$$

4.2.3 Identical bosons

In this case,

$$Q = \prod_{i=1}^{\infty} \frac{(n_i + g_i - 1)!}{n_i!(g_i - 1)!}.$$

4.3 Derivation

In thermal equilibirum, each energy state with some occupying number of particles is equally likely. The most probable configuration is one that can be obtained with the largest number of different ways, such that $Q(n_i)$ is **maximum**. The only constraints in this problem are that the total number of particles in each state add up to the total, or

$$\sum_i n_i = N,$$

and that the total energy is maintained as

$$\sum_i n_i E_i = E_{\text{tot}}.$$

To solve such a problem we can introduce a new function and Lagrange multipliers that help maintain the constraints. Instead of maximizing Q, it's more convenient to consider $\ln Q$. So we want to maximize

$$G = \ln Q + \alpha \left[N - \sum_i n_i \right] + \beta \left[E_{\text{tot}} - \sum_i n_i E_i \right].$$

Then to find the maximum we compute $\partial G / \partial n_j = 0$. Also, regarding the Lagrange multipliers, $\partial G / \partial \alpha = 0$ and $\partial G / \partial \beta = 0$ simply reproduce the constraints.

The quantity Q needs to be considered for the 3 different types of particles that we've discussed.

It will also be helpful to utilize Stirling's approximation:

$$\ln(x!) \approx x \ln x - x, \tag{4.6}$$

which holds when $x \gg 1$.

1. Distinguishable particles. Do this in detail. Using our Q in this case we have

$$\begin{aligned}
G &= \ln N! + \ln \prod_{i=1} \frac{g_i^{n_i}}{n_i!} + \alpha \left[N - \sum_i n_i \right] + \beta \left[E - \sum_i n_i E_i \right] \\
&= \ln N! + \sum_i \ln \frac{g_i^{n_i}}{n_i!} + \alpha \left[N - \sum_i n_i \right] + \beta \left[E - \sum_i n_i E_i \right] \\
&= \ln N! + \sum_i n_i \ln g_i - \sum_i \ln n! + \alpha \left[N - \sum_i n_i \right] + \beta \left[E - \sum_i n_i E_i \right] \\
&= N \ln N - N + \sum_i n_i \ln g_i - \sum_i n_i \ln n_i + \sum_i n_i + \alpha \left[N - \sum_i n_i \right] + \beta \left[E - \sum_i n_i E_i \right].
\end{aligned}$$

Note $E \equiv E_{\text{tot}}$.

Now taking the partial derivative

$$\begin{aligned}
\frac{\partial G}{\partial n_j} &= \ln g_j - \ln n_j - \frac{n_j}{n_j} + 1 - \alpha - \beta E_j = 0 \\
&= \ln g_j - \ln n_j - \alpha - \beta E_j = 0 \\
\ln \frac{g_j}{n_j} &= \alpha + \beta E_j \\
\frac{g_j}{n_j} &= e^{\alpha + \beta E_j} \\
n_j &= g_j e^{-\alpha - \beta E_j}.
\end{aligned}$$

This is the result we are looking for.

2. Fermions. Following the same procedure, we find

$$n_j = \frac{g_j}{\exp(\alpha + \beta E_j) + 1}.$$

3. Bosons. Again, the same procedure yields

$$n_j = \frac{g_j}{\exp(\alpha + \beta E_j) - 1}.$$

To determine what α and β are, one needs to plug the n_j into the constraints and consider some specific total particle number N and energy system E. One then finds that

$$\begin{aligned}
\alpha &= -\frac{\mu}{k_{\mathrm{B}} T}, \\
\beta &= \frac{1}{k_{\mathrm{B}} T},
\end{aligned}$$

where μ is the chemical potential and k_{B} is Boltzmann's constant.