Exercise 16.1. Entropy of Fermi and Bose Gases out of Equilibrium. (Question and comments lifted from Schekochihin)

It is possible to construct the statistical mechanics of quantum ideal gases directly in terms of occupation numbers, using the Gibbs method of constructing the canonical ensemble.

Consider an isolated ensemble of $N \gg 1$ copies of our system (gas in a box, i.e. ideal quantum gas) in good thermal contact with one another, and the particles can move freely between copies. We can treat this system like a microcanonical ensemble. Let N_i be the total number of particles that are in the single-particle state i across this entire microcanonical ensemble. Then the average occupation number of the state i per copy is $\overline{n}_i = N_i/N$. If the macrostate of the microcanonical ensemble is {N_1 particles in state-1, N_2 particles in state-2, ... , N_i particles in state-i, ... } and is made up of $\Omega_N(N_1, N_2, ...)$ number of microstates, then the Gibbs entropy associated with the set of occupation numbers $(\overline{n}_1, \overline{n}_2, ..., \overline{n}_i, ...)$ will be

$S_G(\overline{n}_1, \overline{n}_2, ...) = \frac{1}{N} \ln \Omega_N(N_1, N_2, ...)$

in the limit N $\longrightarrow \infty$ and all $N_i \longrightarrow \infty$ while keeping $\overline{n}_i$ constant.

{This is very similar to the construction in §§8.1.3 or 12.1.3 of the Gibbs entropy of a set of probabilities of microstates, except we now have different rules about how many particles can be in any given microstate i: (i) only at most one particle per state for a fermion gas, and; (ii) any number of particles in any state for a boson gas.

a) Prove that the Gibbs entropy, as defined above, is

$S_G = -\sum_i \overline{n}_i \ln \overline{n}_i \pm (1 \mp \overline{n}_i) \ln(1 \mp \overline{n}_i)$ (16.16)

where the upper sign is for fermions and the lower for bosons.

Hint. The number of microstates of a macrostate $\Omega_N(N_1, N_2, ...)$ can be calculated by counting the number of ways the N_1 particles in the state-1 can be distributed among the N systems, then multiply that by the number of ways the N_2 particles in the state-2 can be distributed, then with the N_3 case, ...

In the fermion case, this is equivalent to solving the number of ways of placing N_i particles into N boxes, where each box can only hold at most 1 particle. (Simple combinatorics.) On the other hand, in the boson case, this is equivalent to solving the number of ways of placing N_i particles into N boxes, where each box can hold arbitrarily many particles. (Use stars and bars method.)

Note that Eq. (16.16) certainly holds for Fermi and Bose gases in equilibrium, i.e., if the occupation numbers $\overline{n}_i$ are given by (16.14), but you have shown now that it also holds out of equilibrium, i.e., for arbitrary sets of occupation numbers (arbitrary particle distributions).

b) Considering a system with fixed mean energy and number of particles and maximising S_G, derive from Eq. (16.16) the Fermi–Dirac and Bose–Einstein formulae (16.14) :

$\overline{n}_i = \frac{1}{e^{\beta(\varepsilon_i - \mu)} \pm 1}$

for the mean occupation numbers in equilibrium.

c) Devise a way to treat a classical ideal gas by the same method.

Post Script:

The machinery you have learned from Exercise 16.1 can be used in a somewhat unexpected way to think of the statistics of self-gravitating systems (e.g., distribution of energies of stars in a galaxy) or of collisionless plasmas (cf. Exercise 6.3)—generally, systems of many particles interacting via some field (gravitational, electromagnetic) but not experiencing particle-on-particle collisions. It turns out one can argue that, subject to certain assumptions, these (classical!) systems strive towards a variant of the Fermi–Dirac distribution known as the Lynden-Bell distribution (after the seminal paper by Lynden-Bell 1967). If you are intrigued by this, read §8.5 of Schekochihin (2020) and do Exercise 8.3 in that section.