## LECTURE 35: IDEAL QUANTUM GASSES Friday, April 17, 2020

Now that we have a new way of labeling states, let's look at the partition function in occupation number representation.

$$Z = \sum_{\{n_{\alpha}\}}^{\sum_{\alpha} n_{\alpha} = N} \prod_{\alpha} e^{-\beta \epsilon_{\alpha} n_{\alpha}}$$

An additional constraint must be made on this sum. For Fermions, we need to consider the Pauli exclusion principle, so the sum will have  $n_{\alpha} \in \{0, 1\}$ , whereas Bosons can have  $n_{\alpha} \in \mathbb{N}$ .

The fixed N constraint is annoying and makes this hard to calculate, but we can remove this constraint by moving to the grand canonical ensemble:

$$\mathcal{Z} = \sum_{N=0}^{\infty} Z_N e^{\beta \mu N}$$

$$= \sum_{N=0}^{\infty} \sum_{\{n_{\alpha}\}}^{\sum_{\alpha} n_{\alpha} = N} \prod_{\alpha} e^{-\beta (\epsilon_{\alpha} - \mu) n_{\alpha}}$$

The interesting thing here is that the first sum makes the constraint  $\sum_{\alpha} n_{\alpha} = N$  superfluous! Since we sum all N up anyway, there is no reason to separate these into groups of fixed N.

$$\mathcal{Z} = \sum_{\{n_{\alpha}\}} \prod_{\alpha} e^{-\beta(\epsilon_{\alpha} - \mu)n_{\alpha}}$$

$$= \sum_{n_{1}} \sum_{n_{2}} \dots \prod_{\alpha} e^{-\beta(\epsilon_{\alpha} - \mu)n_{\alpha}}$$

$$= \sum_{n_{1}} e^{-\beta(\epsilon_{1} - \mu)n_{1}} \sum_{n_{2}} e^{-\beta(\epsilon_{2} - \mu)n_{2}} \dots$$

$$= \prod_{\alpha} \sum_{n_{\alpha}} e^{-\beta(\epsilon_{\alpha} - \mu)n_{\alpha}}$$

Therefore

$$\Omega = -k_B T \ln(\mathcal{Z}) = \begin{cases}
-k_B T \sum_{\alpha} \ln\left(\sum_{n_{\alpha}=0}^{1} e^{-\beta(\epsilon_{\alpha}-\mu)n_{\alpha}}\right) \\
-k_B T \sum_{\alpha} \ln\left(\sum_{n_{\alpha}=0}^{\infty} \left(e^{-\beta(\epsilon_{\alpha}-\mu)}\right)^{n_{\alpha}}\right)
\end{cases}$$

$$= \begin{cases}
-k_B T \sum_{\alpha} \ln\left(1 + e^{-\beta(\epsilon_{\alpha}-\mu)}\right) & \text{Fermions} \\
-k_B T \sum_{\alpha} \ln\left(\frac{1}{1 - e^{-\beta(\epsilon_{\alpha}-\mu)}}\right) & \text{Bosons}
\end{cases}$$

$$= \begin{cases}
-k_B T \sum_{\alpha} \ln\left(1 + e^{-\beta(\epsilon_{\alpha}-\mu)}\right) & \text{Fermions} \\
+k_B T \sum_{\alpha} \ln\left(1 - e^{-\beta(\epsilon_{\alpha}-\mu)}\right) & \text{Bosons}
\end{cases}$$

$$= \mp k_b T \sum_{\alpha} \ln\left(1 \pm e^{-\beta(\epsilon_{\alpha}-\mu)}\right)$$
Bosons

When we use  $\{\mp,\pm\}$  notation, we will always use it in the order in which the Fermion is in the top of the notation and the Boson is in the bottom.

How many particles do we have in a particular state  $\alpha$ ?

$$\langle n_{\alpha} \rangle = \frac{1}{\mathcal{Z}} \left( \prod_{\alpha'} \sum_{n_{\alpha'}} n_{\alpha} e^{-\beta(\epsilon_{\alpha'} - \mu) n_{\alpha'}} \right)$$

$$= \frac{1}{\mathcal{Z}} \left( \prod_{\alpha'} \sum_{n_{\alpha'}} \left( -\frac{1}{\beta} \frac{\partial}{\partial \epsilon_{\alpha}} \right) e^{-\beta(\epsilon_{\alpha'} - \mu) n_{\alpha'}} \right)$$

$$= -\frac{1}{\beta} \frac{1}{\mathcal{Z}} \frac{\partial}{\partial \epsilon_{\alpha}} \mathcal{Z}$$

$$= -\frac{1}{\beta} \frac{\partial}{\partial \epsilon_{\alpha}} \ln(\mathcal{Z}) = \frac{\partial \Omega}{\partial \epsilon_{\alpha}}$$

$$\langle n_{\alpha} \rangle = \frac{\partial}{\partial \epsilon_{\alpha}} \left[ \mp k_{B} T \sum_{\alpha'} \ln \left( 1 \pm e^{-\beta(\epsilon_{\alpha'} - \mu)} \right) \right]$$

$$= \mp k_{B} T \frac{\pm e^{-\beta(\epsilon_{\alpha} - \mu)} (-\beta)}{1 \pm e^{-\beta(\epsilon_{\alpha} - \mu)}}$$

$$= \frac{e^{-\beta(\epsilon_{\alpha} - \mu)}}{1 \pm e^{-\beta(\epsilon_{\alpha} - \mu)}}$$

$$= \frac{1}{e^{\beta(\epsilon_{\alpha} - \mu)} \pm 1} \begin{cases} \text{Fermi} \\ \text{Bose} \end{cases}$$

This expression appears a lot, so we will write it as

$$\langle n_{\alpha} \rangle = \mathcal{F}_{\pm}(\epsilon_{\alpha} - \mu)$$

For large  $\epsilon$ , the function  $\mathcal{F}(\epsilon)$  is just the Boltzmann factor  $e^{-\beta\epsilon}$ , regardless of Fermion or Boson statistics. However, the expectation values are very different for small  $\epsilon$ .

We can write down the density of states for a single particle as

$$D(\epsilon) = \sum_{\alpha} \delta(\epsilon - \epsilon_{\alpha})$$

and the cumulative density of states as

$$W(\epsilon) = \int_{-\infty}^{\epsilon} d\epsilon' D(\epsilon')$$

We can therefore write

$$\Omega = \mp k_B T \int_0^\infty d\epsilon \, D(\epsilon) \ln \left( 1 \pm e^{-\beta(\epsilon - \mu)} \right)$$

Let's do integration by parts, integrating  $D(\epsilon)$  and differentiating the logarithm.

$$\Omega = -\int d\epsilon W(\epsilon) \mathcal{F}_{\pm}(\epsilon - \mu)$$

Therefore,

$$\langle N \rangle = \sum_{\alpha} \langle n_{\alpha} \rangle = \int ddp silon D(\epsilon) \mathcal{F}_{\pm}(\epsilon - \mu) = -\frac{\partial \Omega}{\partial \mu}$$