UCSB, Physics 129L, Computational Physics
Lecture notes, Week 5

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1 Ensembles with indistinguishable particles

1.1 Bosons

While the above discussion is general, particles are distinguishable. Consider an ideal gas composed of N non-interacting (fermionic, bosonic, or classical) particles. In the classical case, the occupation number $n(E)$ at a given energy is directly weighted by the Boltzmann factor,

$$P_{\text{prefer}}(X_i) = \frac{1}{Z}\exp\left(-\frac{E(X_i)}{k_B T}\right), \tag{1}$$

such that $n(E) = NP_{\text{prefer}}(X_i)$.

However, things are different if particles are indistinguishable. Let's consider N non-interacting particles within a fixed volume, each carrying an energy ϵ when moving and has zero energy when stopped (This can be extended further to additional energy levels). Under canonical ensemble, the partition function of the system is given by summing all possible arrangements with state multiplicity $\binom{N}{j}$,

$$Z = \frac{1}{N!}\sum_{j=0}^{N}\binom{N}{j}\exp(-\beta j\epsilon) = \frac{1}{N!}(1+e^{-\beta\epsilon})^N, \qquad P(E = n\epsilon) = \frac{1}{ZN!}\binom{N}{n}\exp(-\beta n\epsilon), \tag{2}$$

where we divide $N!$ since there are N arrangements within. For example, suppose we have a system with $N = 3$ particles, all of which are indistinguishable.

For example, if we want to find the number of ways to place two of these particles in a state with energy ϵ and the third in a different state, using

$$\binom{N}{n} = \binom{3}{2} = 3$$

gives us three configurations:

- First two particles has energy ϵ, third with zero energy.
- First and third has energy ϵ, second with zero energy.
- Second and third has energy ϵ, first with zero energy.

The average number of particles that have zero energy is given by,

$$\begin{aligned} N^C(\text{ground}) &= \sum_{n=0}^{N}(N-n)P(E=n\epsilon) = \frac{1}{ZN!}\sum_{n=0}^{N}(N-n)\binom{N}{n}\exp(-\beta n\epsilon) \\ &= \frac{1}{ZN!}N(1+e^{-\beta\epsilon})^{N-1} = \frac{N}{1+e^{-\beta\epsilon}}. \end{aligned} \tag{3}$$

Note that at high temperature, $\beta \to 0$, we have an average of $N/2$ from the system. Equal-likely to be in the ground state and the excited state.

In **Bose-Einstein statistics**, the state with N particles must be **considered collectively** as a fraction of the states with energy $\epsilon, 2\epsilon, 3\epsilon, \cdots$ (particles within each fraction share the same phase). The partition function is given by,

$$Z = \sum_{j=0}^{N}\exp(-\beta j\epsilon) = \frac{1-e^{-\beta\epsilon(N+1)}}{1-e^{-\beta\epsilon}}, \tag{4}$$

where the number of particles in the ground state is given by,

$$\begin{aligned} N(\text{ground}) &= \sum_{n=0}^{N}(N-n)P(E=n\epsilon) = \frac{1}{Z}\sum_{n=0}^{N}(N-n)\exp(-\beta n\epsilon) \\ &= N - \frac{1}{Z}\frac{\partial Z}{\partial(\beta\epsilon)} = N - \frac{\partial[\ln(Z)]}{\partial(\beta\epsilon)} \\ &= N + \frac{1}{\exp(\beta\epsilon)-1} - \frac{(N+1)}{\exp(\beta\epsilon(N+1))-1} \end{aligned} \tag{5}$$

So far, this equation is not defined when energy is zero since we do not consider any change in energy resulting from changes in particle number. Let's add the "chemical potential", an additional energy term that promote ($\mu < 0$) or demotes ($\mu > 0$) particle grouping. It is global such that it does not depend on specific states. Let's see how much it can collect particles purely based on amount of energy if we give them enough particles,

$$\begin{aligned}\Omega_G &= \sum_{j=0}^{N\to\infty} \exp(-\beta[\epsilon j - \mu j]) = \frac{1-e^{-\beta(\epsilon-\mu)(N+1)}}{1-e^{-\beta(\epsilon-\mu)}} \\ &= \begin{cases} \frac{1}{1-e^{-\beta(\epsilon-\mu)}} & \beta(\mu-\epsilon)<0 \\ \frac{1}{e^{-\beta(\epsilon-\mu)}-1}e^{-\beta(\epsilon-\mu)N} \to \infty & \beta(\mu-\epsilon)>0 \end{cases}.\end{aligned} \tag{6}$$

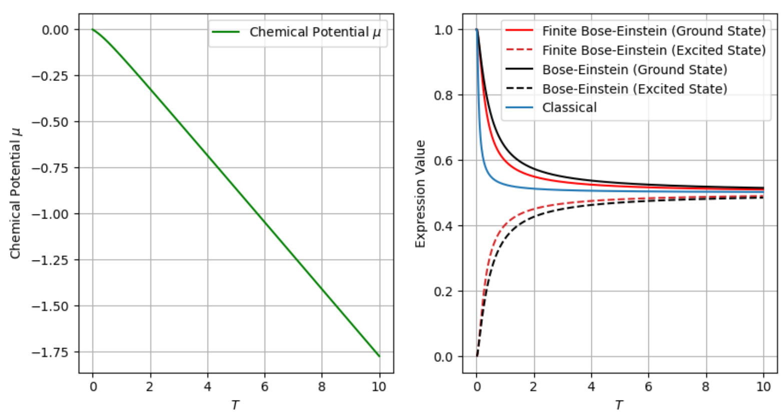
We can see that if $\mu-\epsilon>0$, the partition function goes to infinity, which makes the system non-normalizable (unless population inversion is occurred, $\beta<0$). The average number of particles is given by,

$$\begin{aligned} N(\text{excited state}) &= k_B T \frac{\partial}{\partial\mu}\ln(\Omega_G) = \frac{1}{e^{\beta(\epsilon-\mu)}-1}, \\ N(\text{ground state}) &= k_B T \frac{\partial}{\partial\mu}\ln(\Omega_G) = \frac{1}{e^{\beta(0-\mu)}-1}, \end{aligned} \tag{7}$$

such that,

$$N(\text{excited state}) + N(\text{ground state}) = N. \tag{8}$$

For a fixed N, a larger gap ϵ increases the stability of the ground state populations. You may notice the difference due to finite system size: it can be corrected using the exact expression above. Form the plot, we can see that for finite system, there is a shift in the occupation fraction.



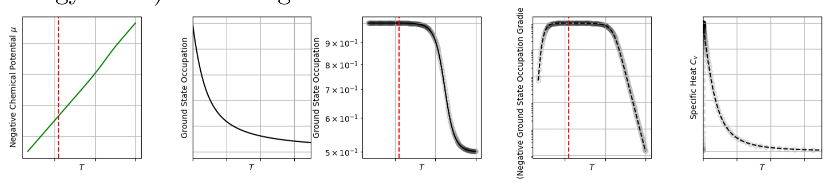
Let's think about the rate of change in the ground state population. This gives by the derivative with respect to the temperature capturing the rate of evaporation of ground state population,

$$R(T) = \frac{\partial N(\text{ground})}{\partial T} \leq 0, \tag{9}$$

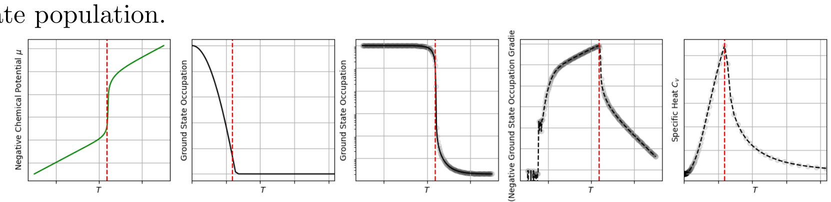
and the **specific heat capacity**,

$$C_V(T) = \frac{\partial E}{\partial T} \geq 0, \tag{10}$$

where we like to find singularity in its derivative, as a traditional signature of BEC. As you can see from the picture below, no BEC occur in a traditional sense. The reason is clear: we do not give the system enough density of states (or energy levels) near the ground state to form BEC.



On the other hand, let's increase the density of states near a thin spectrum above the $E = 0$. As you can see from the picture below, BEC will occur, as identified by the singularity in the derivative, and different behavior in ground state population.



1.2 Fermion

Fermions are particles with half-integer spin (e.g., electrons, protons, neutrons), and they obey the Pauli exclusion principle, which states that no two identical fermions can occupy the same quantum state simultaneously. Let's use the same 2-level system discussed for bosons. In Fermi-Dirac statistics, The state with N particles must be considered collectively as a fraction of the states with $M \geq N$ energy levels $\epsilon, 2\epsilon, 3\epsilon, \cdots M\epsilon$, and the energy is filled one by one until there are N atoms. Therefore, you need to have at least N energy levels to put N atoms in. In fact, the ground state is defined as full occupation of the lowest N energy levels. The partition function is given by (less not considering the spin degenerated case) under canonical ensemble,

$$\begin{aligned} Z &= \left(\sum_{j=0}^{1} \exp(-\beta j\epsilon)\right)\left(\sum_{j=0}^{1} \exp(-2\beta j\epsilon)\right)\cdots\left(\sum_{j=0}^{1} \exp(-\beta M j\epsilon)\right) = \prod_{m=1}^{M} z_m \\ &= \prod_{m=1}^{M} \left(1+\exp(-\beta m\epsilon)\right). \end{aligned} \tag{11}$$

Then, the probability of find a microstate with energy $E = m\epsilon$ is given by,

$$P(E = m\epsilon) = \frac{\exp(-\beta m\epsilon)}{z_m} = \frac{1}{1+e^{\beta m\epsilon}}, \tag{12}$$

and average occupation is simply related to the above probability,

$$N(E = m\epsilon) \sim P(E = m\epsilon). \tag{13}$$

As seem in the exponential, it is trivial for the lowest occupations as it is almost impossible to excite any thing out of the lowest energy state. This is one reason that those energy levels are hide under the **fermi sea**. For this reason, most of time, we do not care them, at least for low energy physics. Let's neglect those below, and introduce a reference point that shifts our focus on somewhere else. The grand canonical ensemble is formulated such that,

$$P(E = m\epsilon) = \frac{\exp(-\beta[m\epsilon - \mu])}{z_m} = \frac{1}{1 + e^{\beta(m\epsilon-\mu)}}, \tag{14}$$

when $\epsilon = \mu$, $P(E = \mu) = 1/2$, which is called fermi-level (or surface).

1.3 A Revisit: Moments, Cumulants, and Ensemble Averages

An analogous concept can be found in statistical physics, which deals with the thermodynamic properties of large ensembles of microstates. In this context, macroscopic physical properties such as temperature, particle number, and energy can be viewed as random variables, depending on ensembles. Consider an ideal gas composed of N non-interacting (fermionic, bosonic, or classical) particles, and we assume there are n_0 numbers of particles that fall within a specific energy range, $E \pm \epsilon$. The probability of finding a particle within the above energy window is given by the ratio,

$$\left(\frac{n_0}{N}\right)_{\text{fermi}} = \frac{g(E)}{e^{(E-\mu)/kT} + 1}, \quad \left(\frac{n_0}{N}\right)_{\text{bose}} = \frac{g(E)}{e^{(E-\mu)/kT} - 1}, \tag{15}$$

and

$$\left(\frac{n_0}{N}\right)_{\text{classical}} = g(E)\frac{e^{-(E_0-\mu)/kT}}{\sum_j e^{-(E_j-\mu)/kT}}, \tag{16}$$

where μ is the chemical potential and $g(E)$ is the density of states (multiplicity around a given energy). The v-th moment as,

$$\langle E^v \rangle = \int_{-\infty}^{\infty} E^v \left(\frac{n_0}{N}\right)_X \mathrm{d}E, \tag{17}$$

where X labels the statistics (fermionic, bosonic, or classical). The expectation value of an observable can be written as the sum moments,

$$\langle A \rangle = \int_{-\infty}^{\infty} A(E) \left(\frac{n_0}{N}\right)_X \mathrm{d}E = \sum_{v=0}^{\infty} A_v \langle E^v \rangle, \tag{18}$$

where A has an power expansion, $A(E) = \sum_{v=0}^{\infty} A_v E^v$.

Let's define the **moment generating function** that is proportional to the system partition function,

$$M(Et) = \sum_E \exp\left([t-\beta]E\right), \quad M(Et)|_{t=0} \sim Z. \tag{19}$$

where t is a small parameter around 0. This treatment is identical to the generation of propagators via the source term in the Legendre transform we discussed previously. The v-th moment is generated by taking v derivatives to the moment generating function,

$$\langle E^v \rangle = \frac{d^v}{dt^v} M(Et)|_{t=0}. \tag{20}$$

This treatment is the statistical basis of many-body perturbation theory and Feynman diagram.

The v-th moment,

$$\langle E^v \rangle \sim (\langle E^{v/2} \rangle)^2 + \langle E^{v/3} \rangle \langle E^{2v/3} \rangle + (\langle E^{v/3} \rangle)^3 + \ldots, \tag{21}$$

contains polynomial powers of lower-order moments, but does not contribute to non-trivial correlations at v-th order. **Cumulants** keep the v-th order variations while subtract all lower-order polynomial contributions. Similar to the moment generating function, cumulants are generated via,

$$\langle K^V \rangle = \frac{d^v}{dt^v} \ln[M(Et)]|_{t=0}, \tag{22}$$

and they correspond to the **connected Feynman diagrams** that are important in higher-order scattering processes.

1.4 Normal Distribution (Gaussian)

Normal distribution (Gaussian) is one of the most important distributions in physics. The normal distribution is given by,

$$p(\mu, \sigma) \sim \exp\left(-\frac{1}{2}\frac{(x-\mu)^2}{\sigma^2}\right), \tag{23}$$

where μ, σ are the mean and standard deviation. The integral,

$$\int_{-\infty}^{\infty} \exp\left(-\frac{1}{2}\frac{(x-\mu)^2}{\sigma^2}\right) dx = \sqrt{\frac{2\pi}{\sigma^2}}. \tag{24}$$

The N-dimensional integral is given by,

$$\int_{-\infty}^{\infty} \prod_{i=1}^{N} dv_i \exp\left(-\frac{1}{2}\mathbf{v}^\dagger \mathbf{A} \mathbf{v} + \mathbf{v}^\dagger \mathbf{w}\right) = (2\pi)^{\frac{N}{2}} \sqrt{\det\left(\mathbf{A}^{-1}\right)} \exp\left(\mathbf{w}^\dagger \mathbf{A}^{-1} \mathbf{w}\right). \tag{25}$$

You will look at those in the problem set 3.