An aside on doing Gaussian integrals

\[ \int_{-\infty}^{\infty} d^3r \ e^{-\frac{r^2}{2\sigma^2}} = 4\pi \int_{0}^{\infty} dr \ r^2 e^{-\frac{r^2}{2\sigma^2}} \] spherical coordinates

\[ \int_{-\infty}^{\infty} d^3r \ r^2 e^{-\frac{r^2}{2\sigma^2}} = 4\pi \int_{0}^{\infty} dr \ r^4 e^{-\frac{r^2}{2\sigma^2}} \]

In Cartesian coords:

\[ \int_{-\infty}^{\infty} d^3r \ e^{-\frac{r^2}{2\sigma^2}} = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz \ e^{-\frac{x^2}{2\sigma^2}} e^{-\frac{y^2}{2\sigma^2}} e^{-\frac{z^2}{2\sigma^2}} \]

\[ = \frac{(4\pi \sigma^2)^{3/2}}{\sqrt{2\pi \sigma^2}} = \frac{(2\pi \sigma^2)^{3/2}}{\sqrt{2\pi}} \]

\[ \int_{-\infty}^{\infty} d^3r \ r^2 e^{-\frac{r^2}{2\sigma^2}} = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz \ (x^2 + y^2 + z^2) e^{-\frac{x^2}{2\sigma^2}} e^{-\frac{y^2}{2\sigma^2}} e^{-\frac{z^2}{2\sigma^2}} \]

all 3 terms contribute equally

\[ = 3 \int_{-\infty}^{\infty} dx \ x^2 e^{-\frac{x^2}{2\sigma^2}} \int_{-\infty}^{\infty} dy \ e^{-\frac{y^2}{2\sigma^2}} \int_{-\infty}^{\infty} dz \ e^{-\frac{z^2}{2\sigma^2}} \]

\[ = 3 \left( \frac{\sigma^2}{\sqrt{2\pi \sigma^2}} \right) \left( \sqrt{2\pi \sigma^2} \right) \left( \sqrt{2\pi \sigma^2} \right) \]

\[ = 3 \sigma^2 (2\pi \sigma^2)^{3/2} = 3 (2\pi)^{3/2} \sigma^5 \]

All you need to remember is

normalized Gaussian \[ \int_{-\infty}^{\infty} dx \ e^{-\frac{x^2}{2\sigma^2}} = 1 \]

\[ \int_{-\infty}^{\infty} dx \ e^{-\frac{x^2}{2\sigma^2}} \ x^2 = \sigma^2 \]
In spherical coordinates

\[ 4\pi \int_0^\infty r^2 e^{-\frac{r^2}{2\sigma^2}} \, dr = (4\pi) \left( \frac{1}{2} \right) \int_{-\infty}^\infty r^2 e^{-\frac{r^2}{2\sigma^2}} \, dr \]

\[ = 2\pi \sigma^2 \cdot \sqrt{2\pi \sigma^2} = (2\pi \sigma^2)^{\frac{3}{2}} \text{ as before} \]

\[ \pi \int_0^\infty r^4 e^{-\frac{r^2}{2\sigma^2}} \, dr \]

would have to either remember the integral or get it into the form \[ \int_{-\infty}^\infty r^2 e^{-\frac{r^2}{2\sigma^2}} \]

by making two integrations by parts.

But even if we don't do integral exactly, we can get the important behavior by a substitution of variables,

\[ x = \frac{r}{\sigma} \Rightarrow \, dr = \sigma \, dx, \quad r = \sigma x \]

Integral is then \[ 4\pi \sigma^5 \int_0^\infty dx \, x^4 e^{-\frac{x^2}{2}} \]

\[ \text{a constant} \]

so we know \[ \int_{-\infty}^\infty r^4 e^{-\frac{r^2}{2\sigma^2}} \sim \sigma^5 \]

--- back to quantum ensembles!
Even though a stationary $\hat{\beta}$ is diagonal in the basis of energy eigenstates, we can always express it in terms of any other complete basis states:

$$\hat{f}_{nm} = \sum_{\alpha\beta} \langle n|\hat{\beta}|m\rangle = \sum_{\alpha} \langle n|\alpha\rangle \langle\alpha|\hat{\beta}|\beta\rangle \langle\beta|m\rangle$$

In this basis, $\hat{\beta}$ need not be diagonal.

This will be useful because we may not know the exact eigenstates for $\hat{H}$. If $\hat{H} = \hat{H}^0 + \hat{H}^1$, we might know the eigenstates of the singular $\hat{H}^0$, but not the full $\hat{H}$. In this case, it may be convenient to express $\hat{\beta}$ in terms of the eigenstates of $\hat{H}^0$ and treat $\hat{H}^1$ as perturbation. In general it is useful to have the above representation for $\hat{\beta}$ and $\langle\xi| = tr(\hat{\beta}\hat{\xi})$ in an operator form that is independent of its representation in any particular basis.

**Microcanonical ensemble:**

$$\hat{\beta} = \sum_{\alpha} |\alpha\rangle \langle\alpha| \quad \text{with} \quad f_{\alpha} = \begin{cases} \text{const} & E \leq E_{\alpha} \leq E+\Delta \\ 0 & \text{otherwise} \end{cases}$$

and $\sum_{\alpha} f_{\alpha} = 1$

**Canonical ensemble:**

$$\hat{\beta} = \sum_{\alpha} |\alpha\rangle \langle\alpha| \quad \text{with} \quad f_{\alpha} = \frac{e^{-\beta E_{\alpha}}}{\Omega_N}$$

where $\Omega_N = \sum_{\alpha} e^{-\beta E_{\alpha}}$
can also write \( Q_N = \sum_x e^{-\beta E_x} = \sum_x \langle x | e^{-\beta \hat{H}} | x \rangle \)

\[ = \text{trace} \left( e^{-\beta \hat{H}} \right) \]

\[ \hat{\psi} = \frac{e^{-\beta \hat{H}}}{Q_N} \]

\[ \langle \hat{x} \rangle = \frac{\text{trace} \left( \hat{x} e^{-\beta \hat{H}} \right)}{\text{trace} \left( e^{-\beta \hat{H}} \right)} \]

**Grand Canonical Ensemble**

Here \( \hat{\psi} \) is an operator in a space that includes wavefunctions with any number of particles \( N \).

\( \hat{\psi} \) should commute with both \( \hat{H} \) (so it is stationary) and with \( \hat{N} \) (so it doesn't mix states with different \( N \)).

\[ \hat{\psi} = \frac{e^{-\beta (\hat{H} - \mu \hat{N})}}{Z} \]

with \( Z = \text{trace} \left( e^{-\beta (\hat{H} - \mu \hat{N})} \right) = \sum_x e^{-\beta (E_x - \mu N_x)} \)

\[ \langle \hat{x} \rangle = \frac{\text{trace} \left( \hat{x} e^{-\beta \hat{H}} e^{\beta \mu \hat{N}} \right)}{\text{trace} \left( e^{-\beta \hat{H}} e^{\beta \mu \hat{N}} \right)} \]

\[ = \sum_{N=0}^{\infty} z^N \langle \hat{x} \rangle_N \frac{Q_N}{z^N Q_N} \]

\[ = \sum_{N=0}^{\infty} z^N Q_N \]
Example: The harmonic oscillator

Suppose we have a single harmonic oscillator. The energy eigenstates are: \( E_n = n \hbar \omega \left( n + \frac{1}{2} \right) \).

The canonical partition function will be:

\[
Q = \sum_n e^{-\beta E_n} = \sum_n e^{-\beta \hbar \omega \left( n + \frac{1}{2} \right)} = e^{-\frac{\hbar \omega}{2z}} \sum_{n=0}^\infty \left( e^{-\beta \hbar \omega} \right)^n
\]

\[
Q = \frac{e^{-\frac{\hbar \omega}{2z}}}{1 - e^{-\beta \hbar \omega}}
\]

\[
\langle E \rangle = -\frac{\partial}{\partial \beta} \ln Q = -\frac{1}{\beta} \left[ -\frac{\hbar \omega}{2} \ln \left( 1 - e^{-\beta \hbar \omega} \right) \right]
\]

\[
= \frac{\hbar \omega}{2} + \frac{\hbar \omega e^{-\beta \hbar \omega}}{1 - e^{-\beta \hbar \omega}} = \frac{\hbar \omega}{2} + \frac{\hbar \omega}{e^{\beta \hbar \omega} - 1}
\]

We could write:

\[
\langle E \rangle = \hbar \omega \left( \langle n \rangle + \frac{1}{2} \right) \quad \text{where} \quad \langle n \rangle \text{ is the average level of occupation of the \hbar \omega},
\]

\[
\Rightarrow \langle n \rangle = \frac{1}{e^{\beta \hbar \omega} - 1}
\]
Quantum Many-particle Systems

N identical particles described by a wavefunction

\[ \psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) \]

where \( \vec{r}_i \) is the position of particle \( i \)

\[ \psi(1, 2, \ldots, N) \]

\( s_i \) is the spin of particle \( i \)

Identical particles \( \Rightarrow \) prob. distribution \(|\psi|^2\) should be symmetric under interchange of any pair of coordinates:

\[ |\psi(i, \ldots, j, \ldots, N)|^2 = |\psi(1, \ldots, j, \ldots, N)|^2 \]

\( \Rightarrow \) two possible symmetries for \( \psi \)

1) \( \psi \) symmetric under pair interchange

\[ \psi(1, \ldots, \hat{i}, \ldots, j, \ldots, N) = \psi(1, \ldots, j, \ldots, \hat{i}, \ldots, N) \]

2) \( \psi \) antisymmetric under pair interchange

\[ \psi(1, \ldots, \hat{i}, \ldots, j, \ldots, N) = -\psi(1, \ldots, j, \ldots, \hat{i}, \ldots, N) \]

(1) = Bose-Einstein statistics - particle called "bosons"
(2) = Fermi-Dirac statistics - particle called "fermions"

For a general permutation \( P \) that interchanges any number of pairs of particles

1) BE \( \Rightarrow \) \( P \psi = \psi \)

2) FD \( \Rightarrow \) \( P \psi = (-1)^p \psi \) where \( p = \# \) pair interchanges

\[ +\psi \text{ for even permutation} \]

\[ -\psi \text{ for odd permutation} \]
BE statistics are for particles with integer spin, \( s = 0, 1, 2, \ldots \)

FD statistics are for particles with half-integer spin, \( s = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots \)

(proved by quantum field theory)

Consider non-interacting particles

\[ H(1,2,3, \ldots, N) = H^{(1)}(1) + H^{(2)}(2) + \ldots + H^{(N)}(N) \]

sum of single particle Hamiltonians

\[ \Rightarrow \psi(1,2,3, \ldots, N) = \phi_1^{(1)}(1) \phi_2^{(2)}(2) \ldots \phi_N^{(N)}(N) \]

where \( \phi_i \) is an eigenstate of single particle \( H^{(i)} \)

with energy \( E_i \).

But \( \psi \) above does not have proper symmetry.

For BE

\[ \Psi = \frac{1}{\sqrt{N_p}} \sum_{P} \psi \left\downarrow \right. \sum \text{ over all permutations } P \]

\[ \left\downarrow \right. \text{ normalization } \]

\[ N_p = \text{# possible permutations of } N \text{ particles} = N! \]

For FD

\[ \Psi = \frac{1}{\sqrt{N_p}} \sum_{P} (-1)^P \psi \]

You can verify that the above symmetrizing operators give

\[ \begin{cases} P_0 \Psi_{BE} = \Psi_{BE} \quad \text{? as desired} \\ P_0 \Psi_{FD} = (-1)^P \Psi_{FD} \end{cases} \]

for any permutation \( P_0 \).
For 4 described by the \( N \) single particle eigenstates \( \phi_{\varepsilon_1}, \phi_{\varepsilon_2}, \ldots, \phi_{\varepsilon_N} \), the total energy is

\[
E = \varepsilon_{\varepsilon_1} + \varepsilon_{\varepsilon_2} + \ldots + \varepsilon_{\varepsilon_N} = \sum_j n_j \varepsilon_j
\]

where \( n_j \) is the number of particles in state \( \phi_j \).

For FD statistics, \( n_j = 0 \) or 1 only possibilities.

This is because of \( \psi(1, 2, \ldots, N) = \phi_1(i)\phi_2(j)\phi_3(k)\ldots\phi_N(l) \)

Then when we construct particles 1 and 2 in same state \( \phi_i \)

\[
\psi_{FD} = \frac{1}{\sqrt{N_p}} \sum (-1)^P \psi
\]

Then for every term in the sum \( \phi_1(i)\phi_2(j)\phi_3(k)\ldots\phi_N(l) \)

There must also be a term \( (-1)^P \phi_1(j)\phi_2(i)\phi_3(k)\ldots\phi_N(l) \)

So these cancel pair by pair

And we find \( \psi_{FD} = 0 \)

\( \Rightarrow \) Pauli Exclusion Principle - no two fermions can

occupy the same state, or no two fermions can have

the same "quantum numbers".

For BE statistics, there is no such restriction

and \( n_j = 0, 1, 2, 3, \ldots \) any integer,

The specification of any non-interacting \( N \) particle quantum state

is given by the occupation numbers \( \{ n_i \} \). Each

set of \( \{ n_i \} \) corresponds to one \( N \)-particle state.