"Free" Systems

These are Hamiltonians where the eigenenergy can be decomposed into the following form:

$$\boxed{E^\alpha = \sum_{i=1}^{L} n_i^\alpha \, \varepsilon_i}$$

n_i^α non-negative integers

L = number of distinct ε_i's (= number of single-particle levels, see below)

This is a remarkable simplification!

Consider, for example a case where $n_i^\alpha = 0$ or 1 only. Using just L values of $\{\varepsilon_i\}$, one can construct 2^L E^αs!

When is this decomposition possible? Although the general answer to this question is not known, the most prominent examples are free systems where $\hat{H}$ takes the form.

$$\hat{H} = \sum_{i=1}^{N} \left[\varepsilon(\hat{p}_i) + V(\hat{x}_i) \right]$$

where $[x_i, p_j] = i\,\delta_{ij}$. The Hamiltonian and N is the number of particles.

is thus separable.

First consider the case of distinguishable particles for such a Hamiltonian.

The Schrodinger eqn is :

$$\hat{H} \psi(r_1, \ldots r_N) = E \psi(r_1, \ldots r_N)$$

Since $\hat{H}$ is separable, the solution is

$$\psi^{\{\alpha\}}(r_1, \ldots r_N) \qquad \{\alpha\} = \{\alpha_1, \ldots \alpha_N\}.$$

$$= u^{\alpha_1}(r_1)\, u^{\alpha_2}(r_2) \ldots u^{\alpha_N}(r_N)$$

where $\psi^{\alpha_i}(x)$ satisfies

$$\boxed{\left[\varepsilon(\hat{p}) + V(\hat{x})\right] \psi^{\alpha_i}(x) = \varepsilon^{\alpha_i}\, u^{\alpha_i}(x)}$$

Thus the first particle with coordinate r_1 is in the single-particle eigenstate u^{α_1}, second one with coordinate r_2 is in eigenstate u^{α_2} and so on.

$\{\alpha_i\}$'s need not be distinct — the particles are distinguished by their coordinate labels already. Also, the number of distinct solns to Eq. 38 is unrelated to N, the number of particles.

The eigenenergy E corresponding to the above wave-f^n is clearly.

$$E = \sum_{i=1}^{N} \varepsilon^{\alpha_i}$$

Example: Two distinguishable particles in a harmonic potential

$$\hat{H} = \frac{P_1^2}{2} + \frac{1}{2} m\omega^2 \hat{x}_1^2 + \frac{P_2^2}{2} + \frac{1}{2} m\omega^2 \hat{x}_2^2$$

Note that there are no cross-terms.

We want to solve the Eigenvalue problem:

$$\hat{H} \,|\varphi\rangle = E\,|\varphi\rangle$$

Explicity, $\left[-\frac{\hbar^2}{2}\frac{d^2}{dx_1^2} + \frac{1}{2} m\omega^2 x_1^2 - \frac{\hbar^2}{2}\frac{d^2}{dx_2^2} + \frac{1}{2} m\omega^2 x_2^2 \right]$

$$\psi(x_1, x_2) = E\, \psi(x_1, x_2)$$

The above differential eqn is separable and the solutions are of the form:

$$\psi^{\alpha_1 \alpha_2}(x_1, x_2) = u^{\alpha_1}(x_1)\, u^{\alpha_2}(x_2)$$

where $u(x)$ is a solution to the differential eqn:

$$\left[-\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2\right] u(x) = \mathcal{E}\, u(x)$$

This is just a single particle harmonic oscillator that we have already solved before. There are an infinite number of solns to this eqn, labeled by integer n.

$$|u\rangle_n = (a^+)^n |0\rangle \quad \text{(not normalized)}$$

where $|0\rangle$ is the ground state $(n=0)$.

Thus, for the original problem, the solutions can be labeled by two integers, one each for each particle.

$$|\varphi\rangle^{n_1,n_2} = |u\rangle_{n_1} \otimes |u\rangle_{n_2}$$

$$\boxed{|\varphi\rangle^{n_1,n_2} = (a_1^+)^{n_1} (a_2^+)^{n_2} |0\rangle \otimes |0\rangle}$$

The eigenenergy is $E^{n_1,n_2} = \hbar\omega(n_1+\frac{1}{2}) + \hbar\omega(n_2+\frac{1}{2})$.

Let's calculate the partition f^n of this system in a canonical ensemble at temperature $T = \beta^{-1}$.

$$Z_{\text{distinguishable}} = \operatorname{Tr} e^{-\beta \hat{H}}$$

$$= \sum_{n_1, n_2 = 0}^{\infty} \langle E^{n_1, n_2} | e^{-\beta \hat{H}} | E^{n_1, n_2} \rangle$$

$$= \sum_{n_1, n_2 = 0}^{\infty} e^{-\beta E^{n_1, n_2}}$$

$$= \sum_{n_1, n_2 = 0}^{\infty} e^{-\beta \left[\hbar\omega\left(n_1 + \frac{1}{2}\right) + \hbar\omega\left(n_2 + \frac{1}{2}\right)\right]}$$

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

$$= \left[\frac{e^{-\frac{\beta\hbar\omega}{2}}}{1 - e^{-\beta\hbar\omega}}\right]^2$$

$$\Rightarrow \boxed{Z_{\text{distinguishable}} = \frac{e^{-\beta\hbar\omega}}{\left[1 - e^{-\beta\hbar\omega}\right]^2}}$$

Now we turn to the main topic, the case of <u>indistinguishable</u> particles. Let's first consider bosons.

<u>Identical</u> Bosons

Given a separable Hamiltonian (in the sense defined above), what is the form of eigenstates?

Clearly, a wave-f^n of the form

$$\psi^{\{\alpha\}}(r_1, \ldots r_N) \qquad \{\alpha\} = \{\alpha_1, \ldots \alpha_N\}.$$

$$= \psi^{\alpha_1}(r_1)\,\psi^{\alpha_2}(r_2) \ldots \psi^{\alpha_N}(r_N)$$

is <u>not</u> OK for bosons. This is because the N particles are clearly distinguished by which orbitals they are in — the first particle is in a single-particle state ψ^{α_1}, the second one in ψ^{α_2} and so on.

The central concept that you must recall is that a bosonic wave-f^n is symmetric under exchange of particles.

The above wave-f^n clearly does not have this property. For example, for a two-particle system, the above wave-f^n is

$$\psi(x_1, x_2) = u^{\alpha_1}(x_1)\, u^{\alpha_2}(x_2)$$

Under exchange $x_1 \leftrightarrow x_2$, and

$$\psi(x_1, x_2) \longrightarrow \psi(x_2, x_1)$$
$$= u^{\alpha_1}(x_2)\, u^{\alpha_2}(x_1)$$
$$\neq \psi(x_1, x_2)$$

(unless $\alpha_1 = \alpha_2$, which is not true in general).

Fortunately, there is a simple trick to remedy this. Just "symmetrize" the wave-f^n. That is, consider:

$$\psi^{sym}(x_1, x_2) = \psi(x_1, x_2) + \psi(x_2, x_1)$$
$$= u^{\alpha_1}(x_1)\, u^{\alpha_2}(x_2) + u^{\alpha_2}(x_1) + u^{\alpha_1}(x_2)$$

$\psi^{sym}(x_1, x_2)$ is clearly symmetric under the exchange operation $x_1 \longleftrightarrow x_2$.

This is the general method for constructing eigenstates of identical bosons for separable Hamiltonians.

To really drive the point home, consider symmetric wf^n of three particles:

$$
\begin{aligned}
\psi^{sym}(x_1, x_2, x_3) &= u^{\alpha_1}(x_1)\, u^{\alpha_2}(x_2)\, u^{\alpha_3}(x_3) \\
&+ u^{\alpha_1}(x_1)\, u^{\alpha_3}(x_2)\, u^{\alpha_2}(x_3) \\
&+ u^{\alpha_1}(x_2)\, u^{\alpha_2}(x_1)\, u^{\alpha_3}(x_3) \\
&+ u^{\alpha_1}(x_2)\, u^{\alpha_2}(x_3)\, u^{\alpha_3}(x_1) \\
&+ u^{\alpha_1}(x_3)\, u^{\alpha_2}(x_1)\, u^{\alpha_3}(x_2) \\
&+ u^{\alpha_1}(x_3)\, u^{\alpha_2}(x_2) + u^{\alpha_3}(x_1)
\end{aligned}
$$

The above wave-f^n is unchanged under exchange of any pair of particles.

Fast way to write down symmetrized wave-f^n s :

Construct matrix M with the entries :

$$M_{ij} = \psi^{\alpha_i}(x_j)$$

In the above example :

$$M = \begin{bmatrix} u^{\alpha_1}(x_1) & u^{\alpha_1}(x_2) & u^{\alpha_1}(x_3) \\ u^{\alpha_2}(x_2) & u^{\alpha_2}(x_2) & u^{\alpha_2}(x_3) \\ u^{\alpha_3}(x_1) & u^{\alpha_3}(x_2) & u^{\alpha_3}(x_3) \end{bmatrix}$$

Write down the determinant of M :

$$\begin{aligned} \det(M) = \; & u^{\alpha_1}(x_1)\, u^{\alpha_2}(x_2)\, u^{\alpha_3}(x_3) \\ & - u^{\alpha_1}(x_1)\, u^{\alpha_2}(x_3)\, u^{\alpha_3}(x_2) \\ & + u^{\alpha_1}(x_2)\, u^{\alpha_2}(x_3)\, u^{\alpha_3}(x_1) \\ & - u^{\alpha_1}(x_2)\, u^{\alpha_2}(x_2)\, u^{\alpha_3}(x_3) \\ & + u^{\alpha_1}(x_3)\, u^{\alpha_2}(x_2)\, u^{\alpha_3}(x_2) \\ & - u^{\alpha_1}(x_3)\, u^{\alpha_2}(x_2)\, u^{\alpha_3}(x_1) \end{aligned}$$

Change all minus signs to plus signs, and we are done ! (Check yourself)

Example: Two indistinguishable bosons in a harmonic potential

$$\hat{H} = \frac{P_1^2}{2} + \frac{1}{2} m\omega^2 \hat{x}_1^2 + \frac{P_2^2}{2} + \frac{1}{2} m\omega^2 \hat{x}_2^2$$

What is the partition f^n ?

The first thing to note is that the single particle eigenstates are unchanged compared to the case of distinguishable particles. But the eigenstates of $\hat{H}$ are of-course different since they must be symmetric under the exchange of the two particles. Based on above discussion,

$$\hat{H}\, |\psi\rangle^{n_1, n_2} = E^{n_1, n_2} |\psi\rangle^{n_1, n_2}$$

$$|\psi\rangle^{n_1, n_2} = \left[(a_1^\dagger)^{n_1} (a_2^\dagger)^{n_2} + (a_1^\dagger)^{n_2} (a_1^\dagger)^{n_1} \right] |0\rangle \otimes |0\rangle$$

Thus, the state $|\psi\rangle^{n_1, n_2}$ is same as $|\psi\rangle^{n_2, n_1}$. $E^{n_1, n_2} = \hbar\omega\left(n_1 + \frac{1}{2} + n_2 + \frac{1}{2}\right)$

Partition f^n:

The calculation is very similar to the case of distinguishable particles, we just have keep in mind that the state $|\psi\rangle^{n_1, n_2}$ and $|\psi\rangle^{n_2, n_1}$ are identical.

$$Z_{boson} = \sum_{n_1, n_2} e^{-\beta\hbar\omega\left(n_1 + \frac{1}{2} + n_2 + \frac{1}{2}\right)}$$

with $(n_1, n_2) \equiv (n_2, n_1)$

$$= \frac{1}{2} \sum_{n_1 \neq n_2} e^{-\beta\hbar\omega\left[n_1 + \frac{1}{2} + n_2 + \frac{1}{2}\right]} + \sum_{n_1 = n_2} e^{-\beta\hbar\omega\left[n_1 + \frac{1}{2} + n_2 + \frac{1}{2}\right]}$$

$$= \frac{1}{2}\left[\sum_{n_1, n_2} e^{-\beta\hbar\omega\left(n_1 + \frac{1}{2} + n_2 + \frac{1}{2}\right)} - \sum_{n_1 = n_2} e^{-\beta\hbar\omega\left(n_1 + \frac{1}{2} + n_2 + \frac{1}{2}\right)}\right] + \sum_{n_1 = n_2} e^{-\beta\hbar\omega\left(n_1 + \frac{1}{2} + n_2 + \frac{1}{2}\right)}$$

$$= \frac{1}{2} Z_{distinguishable} + \frac{1}{2} \sum_{n=0}^{\infty} e^{-\beta\hbar\omega(2n+1)}$$

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