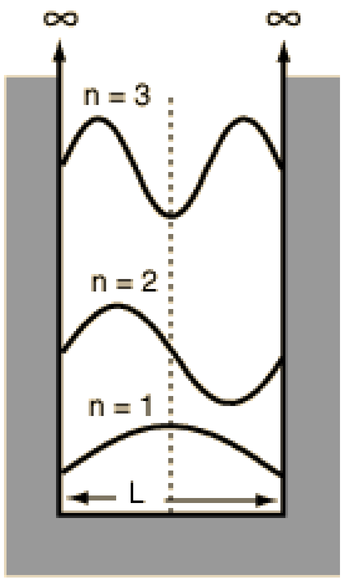
5.4.1 An Example (from book)



x = 0 at left wall of box.

Once again we will consider the infinite square well in 1D.

As opposed to N~10^{23} particles we will have just 3, to do all the proper counting in detail.

We assume they are not interacting i.e.

$$\boxed{E = E_A + E_B + E_C = \frac{\pi^2\hbar^2}{2ma^2}(n_A^2 + n_B^2 + n_C^2)}$$

The quantum numbers n_A, n_B, n_C, are positive integers.

We will assume the total energy is $E = 363(\pi^2\hbar^2/2ma^2)$

This number is larger than the ground state energy because we are in contact with a "bath" at a constant temperature T that provides energy.

Also the weird number 363 is chosen so that there are many possible combinations of integers such that

$$\boxed{n_A^2 + n_B^2 + n_C^2 = 363}$$

In fact, there are 13 combinations of three integers that lead to 363:

(n_A, n_B, n_C)

For classical particles they are all different configurations:

(11, 11, 11).	1 time
(13, 13, 5), (13, 5, 13), (5, 13, 13).	3 times
(1, 1, 19), (1, 19, 1), (19, 1, 1).	3 times
(5, 7, 17), (5, 17, 7), (7, 5, 17), (7, 17, 5), (17, 5, 7), (17, 7, 5)	6 times

Total 13

Each individual state of the square well will have an **occupation number** N_n. A **configuration** is the collection of all occupation numbers of the 3-particle state.

For (11, 11, 11) the configuration is (0,0,0,0,0,0,0,0,0,0,3,0,0,0,0,...)

N_{11} = 3, the rest are 0

For (13, 13, 5), (13, 5, 13), (5, 13, 13) the common configuration is (0,0,0,0,1,0,0,0,0,0,0,0,2,0,0,...)

$N_5 = 1$ $N_{13} = 2$

For (1, 1, 19), (1, 19, 1), (19, 1, 1) the configuration is (2,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,1,0,0...)

$N_1 = 2$ $N_{19} = 1$

For (5, 7, 17), (5, 17, 7), (7, 5, 17), (7, 17, 5), (17, 5, 7), (17, 7, 5) is (0,0,0,0,1,0,1,0,0,0,0,0,0,0,0,0,1,0,0,0,0...)

Most probable configuration: 6 out of 13

$N_5 = 1$ $N_7 = 1$ $N_{17} = 1$

The most probable configuration will be crucial ...

Typical question: selecting a particle at random out of the 3, what is the probably P_n that the chosen one will be in a quantum state "n"?

(11, 11, 11).

(13, 13, 5), (13, 5, 13), (5, 13, 13),

(1, 1, 19), (1, 19, 1), (19, 1, 1),

(5, 7, 17), (5, 17, 7), (7, 5, 17), (7, 17, 5), (17, 5, 7), (17, 7, 5)

For example, for states n=2,3,4,6,8,9,10,12,14,15,16,18,20,21,... the probability is ZERO.

Consider n=1. What is the probability P_1? It appears only in the third line i.e. factor 3/13. In each of the three, the chance is 2/3. Then 3/13 x 2/3 = 2/13.

Consider n=5. What is the probability P_5? It appears in the second line, factor 3/13, and fourth line, factor 6/13. In the second line, each case has chance 1/3. In the fourth line, each case chance 1/3 also. Then answer is 3/13x1/3 + 6/13x1/3 = 3/13.

(11, 11, 11).

(13, 13, 5), (13, 5, 13), (5, 13, 13),

(1, 1, 19), (1, 19, 1), (19, 1, 1),

(5, 7, 17), (5, 17, 7), (7, 5, 17), (7, 17, 5), (17, 5, 7), (17, 7, 5)

Consider n=7. What is P_7? It appears only in the fourth line i.e. factor 6/13. In each of the six, the chance is 1/3. Then 6/13 x 1/3 = 2/13.

Consider n=11. What is P_{11}? It appears in the first line only i.e. factor 1/13. If I am in the first line the chance of a particle in n=11 is 1. Then answer is 1/13x1= 1/13.

Consider n=13. What is P_{13}? It appears in the second line only i.e. factor 3/13. If I am in the second line the chance of a particle in n=13 is 2/3. Then answer is 3/13x2/3= 2/13.

(11, 11, 11).

(13, 13, 5), (13, 5, 13), (5, 13, 13),

(1, 1, 19), (1, 19, 1), (19, 1, 1),

(5, 7, 17), (5, 17, 7), (7, 5, 17), (7, 17, 5), (17, 5, 7), (17, 7, 5)

Consider n=17. What is P_{17}? It appears only in the fourth line i.e. factor 6/13. In each of the six, the chance is 1/3. Then 6/13 x 1/3 = 2/13.

Consider n=19. What is P_{19}? It appears in the third line only i.e. factor 3/13. If I am in the third line the chance of a particle in n=19 is 1/3. Then answer is 3/13x1/3 = 1/13.

End of torture ….

One way to check that all is fine is to add the probabilities. They have to add to 1:

$$P_1 + P_5 + P_7 + P_{11} + P_{13} + P_{17} + P_{19} = \frac{2}{13} + \frac{3}{13} + \frac{2}{13} + \frac{1}{13} + \frac{2}{13} + \frac{2}{13} + \frac{1}{13} = 1$$

For **identical fermions** all is much easier!

(n_A, n_B, n_C)

$(11, 11, 11)$.	out
$(13, 13, 5)$, $(13, 5, 13)$, $(5, 13, 13)$.	out
$(1, 1, 19)$, $(1, 19, 1)$, $(19, 1, 1)$.	out
$(5, 7, 17)$, $(5, 17, 7)$, $(7, 5, 17)$, $(7, 17, 5)$, $(17, 5, 7)$, $(17, 7, 5)$	1 time

P_5=1x1/3=1/3, P_7=1x1/3=1/3, P_{17}=1x1/3=1/3

Total 1

$P_5 + P_7 + P_{17} = 1$

For **identical bosons** not too hard:

(n_A, n_B, n_C)

(11, 11, 11).	1 time
(13, 13, 5), (13, 5, 13), (5, 13, 13).	1 time
(1, 1, 19), (1, 19, 1), (19, 1, 1).	1 time
(5, 7, 17), (5, 17, 7), (7, 5, 17), (7, 17, 5), (17, 5, 7), (17, 7, 5)	1 time

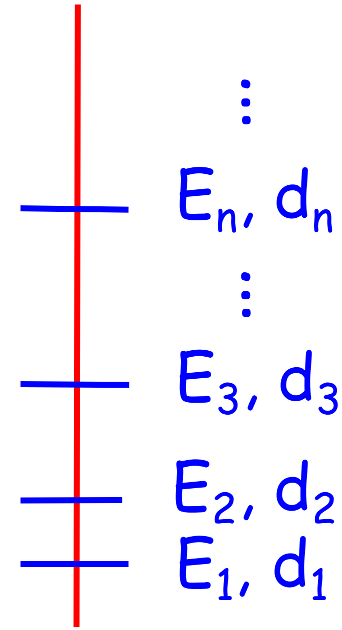
Total 4

P_1 = 1/4x2/3=2/12, P_5=1/4x1/3 + 1/4x1/3=2/12,
P_7 = 1/4x1/3 =1/12, P_{11}=1/4x1=1/4=3/12,
P_{13} = 1/4x2/3 =2/12, P_{17}=1/4x1/3=1/12,
P_{19} = 1/4x1/3 =1/12

$P_1 + P_5 + P_7 + P_{11} + P_{13} + P_{17} + P_{19} =$
2/12+2/12+ 1/12+3/12+2/12+1/12+1/12 = 1

Amazingly, for many many particles N, the math will simplify because **the most probable configuration will totally dominate over the rest**. For example, for classical particles the last configuration (5,7,17) … would be the only one to consider.

5.4.2 The General Case



Consider an arbitrary potential V(x) and assume we know the properties of the one particle states i.e. its energies E_1, E_2, …, E_n, … and the degeneracy of each energy d_1, d_2 , …, d_n, …

Suppose a fixed number of particles N.
In the previous example N=3.

Suppose now I want to investigate a particular configuration (N_1, N_2, …, N_n, …) such that the sum $N_1 + N_2 + \ldots + N_n \ldots = N$.

Given a set of occupations $(N_1, N_2, \ldots, N_n, \ldots)$ we want to know in how many ways $Q(N_1, N_2, \ldots, N_n, \ldots)$ we can get that set, such that the sum $N_1 + N_2 + \ldots + N_n \ldots = N$.

Distinguishable particles first:

In the last lecture (0,0,0,0,1,0,1,0,0,0,0,0,0,0,0,1,0,0,0,0…) appeared 5 times thus Q(0,0,0,0,1,0,1,0,0,0,0,0,0,0,0,1,0,0,0,0…)=6
The configuration (0,0,0,0,0,0,0,0,0,0,3,0,0,0,0,0,0,0,0,0…) appeared only 1 time thus Q=(0,0,0,0,0,0,0,0,0,0,3,0,0,0,0,0,0,0,0,0…)=1.

(11, 11, 11).

(13, 13, 5), (13, 5, 13), (5, 13, 13).

(1, 1, 19), (1, 19, 1), (19, 1, 1).

(5, 7, 17), (5, 17, 7), (7, 5, 17), (7, 17, 5), (17, 5, 7), (17, 7, 5)

We aim to get a generic formula for the "6" and the "1" in the example above.

Here I will give you the results without derivation, and confirm the formulas using the example of last lecture. For full derivation, read book. For distinguishable particles the answer is:

$$\boxed{Q(N_1, N_2, N_3, \ldots) = N! \prod_{n=1}^{\infty} \frac{d_n^{N_n}}{N_n!}}$$

In the example of last lecture, the degeneracy d_n was always 1, so that does not count since $1^{N_n} = 1$. Also N!=3.2.1=6 because we had 3 particles.

For the configuration (0,0,0,0,1,0,1,0,0,0,0,0,0,0,0,1,0,0,0,0…) the eq. says Q(0,0,0,0,1,0,1,0,0,0,0,0,0,0,0,1,0,0,0,0…) = 3!/1!1!1! = 6 (correct).

For the configuration (0,0,0,0,0,0,0,0,0,0,3,0,0,0,0,0,0,0,0,0…) the eq. says Q(0,0,0,0,0,0,0,0,0,0,3,0,0,0,0,0,0,0,0,0…)= 3!/3! = 1 (correct).

For identical fermions it is easier. The answer is:

$$Q(N_1, N_2, N_3, \ldots) = \prod_{n=1}^{\infty} \frac{d_n!}{N_n!(d_n - N_n)!}$$

For the configuration (0,0,0,0,1,0,1,0,0,0,0,0,0,0,0,0,1,0,0,0,0…) the eq. says Q(0,0,0,0,1,0,1,0,0,0,0,0,0,0,0,0,1,0,0,0,0…) = 1!1!1!/1!(1-1)!1!(1-1)!1!(1-1)! = 1 (correct for fermions).

For the configuration (0,0,0,0,0,0,0,0,0,0,3,0,0,0,0,0,0,0,0,0…) the eq. says Q (0,0,0,0,0,0,0,0,0,0,3,0,0,0,0,0,0,0,0,0…) = 0 (correct for fermions) because I cannot place 3 particles in the same state.

For identical bosons the answer is:

$$\boxed{Q(N_1, N_2, N_3, \ldots) = \prod_{n=1}^{\infty} \frac{(N_n + d_n - 1)!}{N_n!(d_n - 1)!}}$$

For the configuration (0,0,0,0,1,0,1,0,0,0,0,0,0,0,0,0,1,0,0,0,0…) the eq. says Q(0,0,0,0,1,0,1,0,0,0,0,0,0,0,0,0,1,0,0,0,0…) = (1+1-1)!(1+1-1)!(1+1-1)!/[1!(1-1)!1!(1-1)!1!(1-1)!] = 1 (correct for bosons).

For the configuration (0,0,0,0,0,0,0,0,0,0,3,0,0,0,0,0,0,0,0,0…) the eq. says Q(0,0,0,0,0,0,0,0,0,0,3,0,0,0,0,0,0,0,0,0…) = (3+1-1)!/3!(1-1)! = 1 (correct for bosons).