PERMUTATIONS & COMBINATIONS

Suppose that we have a collection of n words. (These are assumed to be distinct at this stage.) The number of arrangements or permutations (disregarding questions of syntax) is

$$\boxed{\#\ \text{permutations} = n(n-1)(n-2)\ldots = n!} \tag{1}$$

If only $m<n$ of these words are used then

$$\#\ \text{permutations}\ (m<n) = \underbrace{n(n-1)(n-2)\ldots(n-[m-1])}_{m\ \text{terms}} = n(n-1)\ldots(n-m+1)$$

$$= \frac{n(n-1)\cdots(n-m+1)\cdot(n-m)(n-m-1)\ldots3\cdot2\cdot1}{(n-m)(n-m-1)\ldots3\cdot2\cdot1} = \frac{n!}{(n-m)!} \tag{2}$$

In the above example the sequence of words is important, since we want to distinguish between $W_1W_2W_3$ (where W_i are words) and $W_1W_3W_2$, etc. However, if we were not concerned about the sequence, but merely about which words were used, then we are asking how many combinations can be formed using m words selected from n possibilities.

Example: Returning to Eq. (2) we see that this equation counts as separate the contributions $W_1W_2W_3$, $W_1W_3W_2$, $W_2W_1W_3$, $W_2W_3W_1$, $W_3W_1W_2$, and $W_3W_2W_1$. There are clearly $m! = 3!$ such arrangements. If we do not wish to consider these as distinguishable then we must reduce the result in (2) by $m!$ This gives:

$$\boxed{\begin{array}{l}\text{number of combinations of } n \text{ things taken } m \text{ at a time} \equiv \binom{n}{m} = \dfrac{n!}{m!(n-m)!} \\ \equiv \text{BINOMIAL COEFFICIENT}\end{array}} \tag{3}$$

The expression $\binom{n}{m}$ is called the binomial coefficient because it arises in the binomial expansion

$$(a+b)^n = a^n + \binom{n}{1} a^{n-1} b + \binom{n}{2} a^{n-2} b^2 + \binom{n}{3} a^{n-3} b^3 + \dots + b^n \tag{4}$$

Other Related Questions:

Suppose we have a box with n_1 copies of the word W_1, n_2 copies of W_2, ... with $n_1 + n_2 + n_3 + \dots = n$. We then extract the words from the box one at a time. Question: How many distinguishably different sentences can be formed in this way?

Answer: If all the words were different there would be $n!$ sentences. But since there are $n_i!$ ways of arranging W_i which would produce the same sentence the result is

$$\boxed{\#\text{ of different sentences} = \frac{n!}{n_1!\, n_2!\, n_3! \cdots}} \tag{5}$$

We will use this result below to derive the MAXWELL-BOLTZMANN distribution.

THE BINOMIAL DISTRIBUTION

Binomial Distribution (exact)

Improbable Events | Highly Probable Events

Poisson Distribution (approximate) | Gaussian Distribution (approximate)

Binomial Distribution

Suppose that a fair coin is flipped n times. We want to find the probability that $m \leq n$ heads (h) will be found.

Solution: The results of n-flips can be represented by a sequence of n letters,

$$\underbrace{h\,h\,t\,h\,t\,t\,\ldots\,h}_{n\text{-letters}} \tag{1}$$

In the more general case where the probability of heads $= p$ and the probability of tails is $q = 1-p$ then the probability of any specific sequence is

$$\begin{array}{ccccccccccccc} & & h & h & t & h & t & t & \ldots & h & & & \\ & & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & & \downarrow & & & \\ \text{Prob} & = & p \times & p \times & q \times & p \times & q \times & q & \ldots & \times p & = & p^m q^{n-m} & \end{array} \tag{2}$$

Note that the result in (2) is the same result for any sequence containing m heads and $(n-m)$ tails. Hence the total probability of getting m heads is

$$\text{total prob} = p^m q^{n-m} \otimes \{\text{number of favorable sequences with } m \text{ heads}\} \tag{3}$$

To Clarify: The result in (2) is the probability of getting the specific sequence shown. But we do not care about the sequence, only about the final number of heads m.

To compute the number of favorable sequences containing m heads we note that this number is determined as soon as we determine the positions in the sequence of the m letters h (since the remaining $[n-m]$ letters must be t). So the question comes down to <u>how many ways can we place the m letters h into the n places in the sequence?</u>

<u>Answer:</u> The first h can be placed in n places. The 2ND letter can then be placed in $(n-1)$ places, ... The m-th letter can be placed in $[n-(m-1)]$ places. Hence

$$\#\text{ favorable sequences} \sim \underbrace{n(n-1)(n-2)\cdots(n-m+1)}_{m\text{ factors}} = \frac{n(n-1)\cdots(n-m+1)(n-m)\cdots 3\cdot 2\cdot 1}{(n-m)\cdots 3\cdot 2\cdot 1}$$

$$= \frac{n!}{(n-m)!} \qquad (4)$$

This is <u>almost</u> the right answer, but not quite: In the result in (4) we are counting as distinct sequences $h_2 h_5 h_8$, $h_8 h_5 h_2$, $h_5 h_2 h_8, \ldots$ where h_i denotes a head in the ith position. For m heads there are clearly $m!$ such sequences which are equivalent for our purposes. Hence we must reduce the result in (4) by the number of equivalent sequences which is $m!$ Hence altogether:

$$\boxed{\#\text{ of favorable sequences} = \frac{n!}{m!(n-m)!} = \binom{n}{m}} = \text{BINOMIAL COEFFICIENT} \qquad (5)$$

<u>Example:</u> How many sequences give 2 heads & 1 tail in 3 tosses?

<u>TOSSES</u>: →	I	II	III
	h	h'	t
	h'	h	t
	t	h	h'
	t	h'	h
	h	t	h'
	h'	t	h

$h \neq h' \Rightarrow \dfrac{n!}{(n-m)!} = 6$ sequences

$h = h' \Rightarrow \dfrac{n!}{m!(n-m)!} = 3$ sequences

Collecting the previous results together we find

$$\boxed{P(m) = \text{total probability of } m \text{ heads} = p^m q^{n-m}\binom{n}{m} = p^m (1-p)^{n-m}\binom{n}{m}} \qquad (6)$$

BINOMIAL DISTRIBUTION

Gives the probability of m successes after n-trials if the probability for success is p, and for failure is $q = 1-p$.

Example: What is the probability that the number 1 will appear exactly 4 times in the course of 10 throws of a die?

Solution: Here $p = 1/6$, $1-p = 5/6$, $n = 10$, $m = 4$

Then $$P(4) = (1/6)^4 (5/6)^{10-4} \binom{10}{4} \qquad (7)$$

$$\binom{10}{4} = \frac{10!}{4!\,6!} = \frac{10\cdot 9\cdot 8\cdot 7\cdot \cancel{6\cdot 5\cdot 4\cdot 3\cdot 2\cdot 1}}{(4\cdot 3\cdot 2\cdot 1)\,\cancel{(6\cdot 5\cdot 4\cdot 3\cdot 2\cdot 1)}} = 210 \qquad (8)$$

Combining (7) & (8): $P(4) = (1/6)^4 (5/6)^6 \times 210 = 0.0543$

The binomial distribution (as a function of m) is then specified by 2 input parameters p and n, which determine its shape. Some sketches of the binomial distribution for different choices of p & n are given on the next page.

THE MAXWELL-BOLTZMANN DISTRIBUTION

See GLASSTONE - "Theoretical Chemistry" p. 286 ff

This is simultaneously an application of permutations, combinations, Lagrange multipliers, and Stirling's Formula

Consider a gas containing n atoms or molecules. For simplicity we consider the case where the atoms are point objects described by coordinates $\vec{q}_j$ and momenta $\vec{p}_j$ $(j = 1, \ldots n)$. Each atom can be described by a point in phase space $(q_{j1}, q_{j2}, q_{j3}, p_{j1}, p_{j2}, p_{j3})$. If we suppress the index j temporarily then if q_1 is in the range q_1 to $q_1 + dq_1 \equiv (q_1 + \delta q_1)$, etc. then the volume δv in phase space occupied by this atom is

$$\delta v = \delta q_1 \delta q_2 \delta q_3 \delta p_1 \delta p_2 \delta p_3 \equiv \text{cell in phase space} \qquad (1)$$

This is the case for one atom or molecule.

More generally we can write $\delta v \longrightarrow \delta v_{i(j)}$ where the notation means that the jth molecule occupies the ith cell in phase space.

Combinatorics: The state of a collection of atoms can then be specified by asking how we can distribute the n atoms of a sample such that there are n_1 in cell δv_1, n_2 in cell δv_2, ... etc. The number of ways this can be done $\equiv G$ can be found from our previous discussion. Clearly G is given by

$$\boxed{G = \frac{n!}{n_1!\, n_2! \ldots n_i!}} \qquad (2)$$

This is Eq. (5) on p. 153: $G \leftrightarrow$ # of sentences; all atoms in the same cell are equivalent:

Stated another way: We are saying in a sense that the situation when n_1 words are $w_1, \ldots$ is the same as saying that n_1 atoms are in the phase-space volume δv_1.

Now the n atoms can be distributed in many ways such that $\sum_j n_j = n$. We then invoke one of the basic assumptions of statistical mechanics that the probability W that the system will be in a certain configuration (specified by $\{n_j\}$) is proportional to G computed for that configuration:

$$W = \text{Constant} \otimes G \equiv cG \tag{3}$$

The most likely configuration is then the one that maximizes W. To find out what configuration this is consider $\ln W$

$$\ln W = \ln c + \ln n! - \sum_i \ln (n_i!) \tag{4}$$

Use the Stirling Formula : $n! \cong \sqrt{2\pi n}\; n^n e^{-n}$ (5)

Approximately then, $\ln(n!) \cong \ln\sqrt{2\pi} + \ln(n^{1/2}) + n\ln n - n$ (6)

$$\therefore \boxed{\ln(n!) \cong n\ln n - n} \tag{7}$$

Hence: $\ln W \cong \ln c + (n\ln n - n) - \sum_i (n_i \ln n_i - n_i)$

$$= \ln c + (n\ln n \cancel{-n}) - \sum_i n_i \ln n_i + \underbrace{\cancel{\sum_i n_i}}_{n} \tag{8}$$

Hence: $\boxed{\ln W \cong \ln c + n\ln n - \sum_i n_i \ln n_i}$ (9)

We want to extremize (here maximize) W as a function of the n_i. So we consider:

$$\delta(\ln W) = \underbrace{\delta(\ln c)}_{= 0} + \underbrace{\delta(n\ln n)}_{= 0\ (n = \text{fixed})} - \delta\Big(\sum_i n_i \ln n_i\Big) \tag{10}$$

It follows from (10) that

$$0 \equiv \delta(\ln W) = -\sum_i \left(n_i \frac{1}{n_i} + \ln n_i\right)\delta n_i \Rightarrow \sum_i (1+\ln n_i)\,\delta n_i = 0 \qquad (11)$$

We wish to carry out this extremization subject to the constraints:

$$\sum_i n_i = n \Rightarrow \alpha \sum_i \delta n_i = 0 \qquad ; \; n = \text{total \# of atoms}$$

$$\sum_i \epsilon_i n_i = E \Rightarrow \beta \sum_i \epsilon_i \delta n_i = 0 \qquad E = \text{total energy of atoms}$$

$$(12)$$

α, β are <u>Lagrange multipliers</u>

Combining (11) & (12) we find: $\sum_i (1 + \ln n_i + \alpha + \beta\epsilon_i)\,\delta n_i = 0$

Having introduced α and β we can now argue that <u>the δn_i are arbitrary</u> since they are not constrained any longer by (12). Since the δn_i are arbitrary we can then argue that the coefficient of each δn_i must separately vanish. This gives:

$$1 + \ln n_i + \alpha + \beta\epsilon_i = 0 \Rightarrow \ln n_i = \underbrace{(-1-\alpha)}_{\text{another constant}-\alpha' \rightarrow \text{ rename as } -\alpha} - \beta\epsilon_i \qquad (13)$$

sign is conventional

$$\therefore \ln n_i = -\alpha - \beta\epsilon_i$$

$$\Rightarrow n_i = \underbrace{e^{-\alpha}}_{\text{normalization constant}} e^{-\beta\epsilon_i} \Rightarrow \boxed{n_i(\epsilon_i) = \text{Const}\; e^{-\beta\epsilon_i}} \qquad (14)$$

By comparing to the usual macroscopic ideal gas laws we can then deduce that $\beta = 1/k_B T$. So finally

$$\boxed{n_i(\epsilon_i) = \text{Const}\; e^{-\epsilon_i/k_B T}} \qquad (15)$$

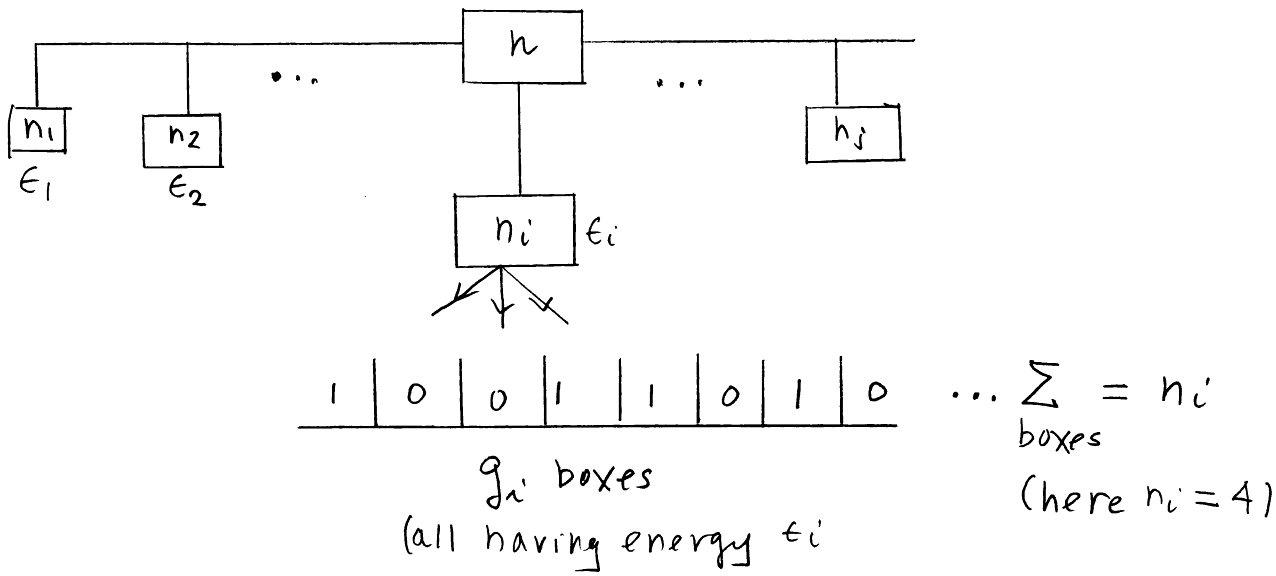
<u>MAXWELL-BOLTZMANN DISTRIBUTION</u>

THE FERMI–DIRAC DISTRIBUTION

This is another example of the use of combinatorics, but now applied to a quantum system. As in the Maxwell–Boltzmann case we assume a collection of particles (now fermions) obeying the PAULI EXCLUSION PRINCIPLE. This is a fundamental change in doing the combinatorics. The constraints are, as before:

$$\boxed{\sum_i n_i = n \qquad ; \qquad \sum_i \epsilon_i n_i = E} \qquad (1)$$

The combinatoric problem can be expressed in terms of a tree graph:



The different "boxes" represent possible degenerate states: States having different quantum numbers, but the same energy ϵ_i. By virtue of the Pauli Exclusion Principle, there can be at most one fermion/state so the "occupation number" of each state is either 0 or 1. Clearly,

$$\boxed{g_i \geqslant n_i} \qquad (2)$$

otherwise >1 particles would be in some boxes.

There is a formal analogy between the analysis for the Fermi-Dirac distribution, and the binomial distribution of a series of coin tosses:

F-D Distribution	Coin Tosses
g_i boxes	g_i tosses
$n_i \leq g_i$ occupied boxes	$n_i \leq g_i$ heads
$(g_i - n_i)$ unoccupied boxes	$(g_i - n_i)$ tails

From the discussion of the binomial distribution, and the picture on the previous page, the number of microscopic states can be determined by asking how many ways can n_i 1's be placed in g_i boxes? [Recall that once the 1's are positioned, the locations of the 0's are fixed.]

The first 1 can be placed in g_i boxes; by virtue of the PAULI EXCLUSION PRINCIPLE the next 1 cannot be placed in the same box, so it has $(g_i - 1)$ choices, ... etc.

Altogether, the number of ways that the n_i 1's can be arranged is then

$$\underbrace{g_i(g_i-1)(g_i-2)(g_i-3)\ldots}_{n_i \text{ factors}} = g_i(g_i-1)(g_i-2)\ldots(g_i-(n-1)) = \frac{g_i!}{(g_i-n_i)!} \tag{3}$$

This is not yet the full answer, just as in the case of the binomial distribution: The result in (3) counts as distinct the configuration $1_3\, 1_5$ (1 in box 3 and 1 in box 5) as well as $1_5\, 1_3$. However, physically these are the same configuration. Thus to prevent this kind of overcounting we must reduce the number in (3) by $n!$ This leads to

Number of "favorable" possibilities for placing n_i particles in g_i "boxes" (all with energy E_i) $\equiv G_i$ is

$$\boxed{G_i = \frac{g_i!}{n_i!\,(g_i - n_i)!} = \binom{g_i}{n_i} = \text{binomial coefficient}} \tag{4}$$

This described the number of possibilities for the states having energy ϵ_i. For a quantum system there will be many such (discrete) states, and hence the total number of possibilities G is given by

$$G = \frac{g_1!}{n_1!(g_1-n_1)!} \otimes \frac{g_2!}{n_2!(g_2-n_2)!} \otimes \cdots \otimes \frac{g_i!}{n_i!(g_i-n_i)!} = \prod_i \frac{g_i!}{n_i!(g_i-n_i)!} \tag{5}$$

As in the previous case of the <u>MAXWELL</u>-<u>BOLTZMANN</u> distribution, the probability of realizing a given macroscopic state where the n particles have been distributed as $n = (n_1, n_2, \ldots, n_i, \ldots)$ is

$$W = (\text{const}) \otimes G \tag{6}$$

To find out what the most likely distribution is we evaluate $\ln W$:

$$\ln W = \ln C + \sum_i \ln\left[\frac{g_i!}{n_i!(g_i-n_i)!}\right] = \ln C + \sum_i \left\{\ln g_i! - \ln n_i! - \ln (g_i-n_i)!\right\} \tag{7}$$

We use the approximation (STIRLING'S FORMULA): $\ln g_i! \cong g_i \ln g_i - g_i$ (8)

From (7) & (8):

$$\ln W \cong \ln C + \sum_i \left\{(g_i \ln g_i - \cancel{g_i}) - (n_i \ln n_i - \cancel{n_i}) - \left[(g_i-n_i)\ln(g_i-n_i) - (\cancel{g_i} - \cancel{n_i})\right]\right\} \tag{9}$$

$$\ln W \cong \ln C + \sum_i \left\{g_i \ln g_i - n_i \ln n_i - (g_i-n_i)\ln(g_i-n_i)\right\} \tag{10}$$

As in the M-B case we can form the function F which incorporates the constraints in terms of the Lagrange multipliers α and β:

$$F = \ln C + \sum_i \left\{ g_i \ln g_i - n_i \ln n_i - (g_i - n_i)\ln(g_i - n_i) \right\} + (-\alpha)\left(\sum_i n_i - n\right) + (-\beta)\left(\sum_i \epsilon_i n_i - E\right) \quad (11)$$

The signs of α & β are purely conventional.

Hence
$$\frac{\delta F}{\delta n_i} = \sum_i \left\{ \cancel{-n_i \frac{1}{n_i}} - \ln n_i \cancel{-(g_i - n_i)\frac{(-1)}{(g_i - n_i)}} + \ln(g_i - n_i) - \alpha - \beta \epsilon_i \right\} = 0 \quad (12)$$

Since the δn_i are now independent the expression in $\{\ldots\}$ must vanish, giving

$$\ln\left(\frac{g_i - n_i}{n_i}\right) = \ln\left(\frac{g_i}{n_i} - 1\right) = \alpha + \beta \epsilon_i \quad (13)$$

Exponentiating: $$e^{\ell(\ldots)} = (\ldots) = \frac{g_i}{n_i} - 1 = e^{\alpha + \beta \epsilon_i} \quad (14)$$

Hence $$\frac{g_i}{n_i} = e^{\alpha + \beta \epsilon_i} + 1 \Rightarrow \boxed{n_i = \frac{g_i}{e^{\alpha + \beta \epsilon_i} + 1}} \quad (15)$$

FERMI-DIRAC DISTRIBUTION

→ Classical Limit: In the classical limit (e.g. at high temperatures) $g_i/n_i \gg 1$ which means that there are many more available states than there are particles to fill them. From the first part of (15) we then see that in the classical limit

$$g_i/n_i \cong e^{\alpha + \beta \epsilon_i} \Rightarrow \boxed{n_i = \frac{g_i}{e^{\alpha + \beta \epsilon_i}}} \quad (16)$$

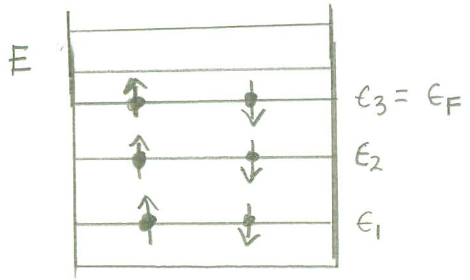
MAXWELL-BOLTZMANN DISTRIBUTION

Hence, as expected the F-D distribution → M-B distribution in the classical limit. For this reason, we can determine β in (15) to be the same as in the M-B distribution,

$$\beta = 1/k_B T \quad (17)$$

In the F-D distribution the constant α is important and is related to the Fermi-Energy ϵ_F:

At $T=0$:



All states up to (and including) ϵ_F are fully occupied, and all states above ϵ_F are un-occupied

We claim that this situation can be described mathematically by Eqs. (16) & (17) if we choose $\boxed{\alpha = -\epsilon_F/k_B T}$. Then

$$\boxed{n_i = \frac{g_i}{e^{(\epsilon_i - \epsilon_F)/k_B T} + 1}} \qquad (18)$$

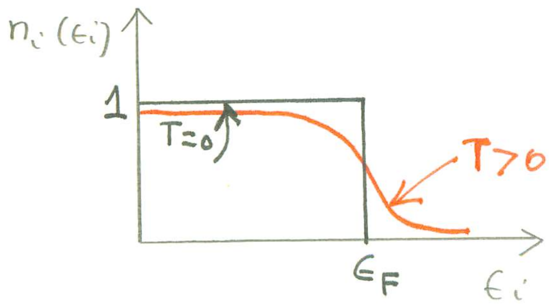
FINAL FORM OF FERMI-DIRAC DISTRIBUTION

To see how this equation reproduces the above figure at $T=0$ we note that:

$$(\epsilon_i - \epsilon_F) > 0 \Rightarrow \frac{1}{e^{(\epsilon_i-\epsilon_F)/k_B T}+1} \xrightarrow{T=0} \frac{1}{e^{+\infty}+1} = 0$$

$$(\epsilon_i - \epsilon_F) < 0 \Rightarrow \frac{1}{e^{(\epsilon_i-\epsilon_F)/k_B T}+1} \xrightarrow{T=0} \frac{1}{e^{-\infty}+1} = 1$$

Pictorially the function in (18) then looks like:



THE BOSE-EINSTEIN DISTRIBUTION

We have n-bosons in a 1-dimensional box, which has allowed discrete energy levels ϵ_i. There are n_i bosons in each energy level with $\sum_i n_i = n$. The B-E distribution answers the question: What are the relative populations of the $n_i = n_i(\epsilon_i)$ as a function of ϵ_i?

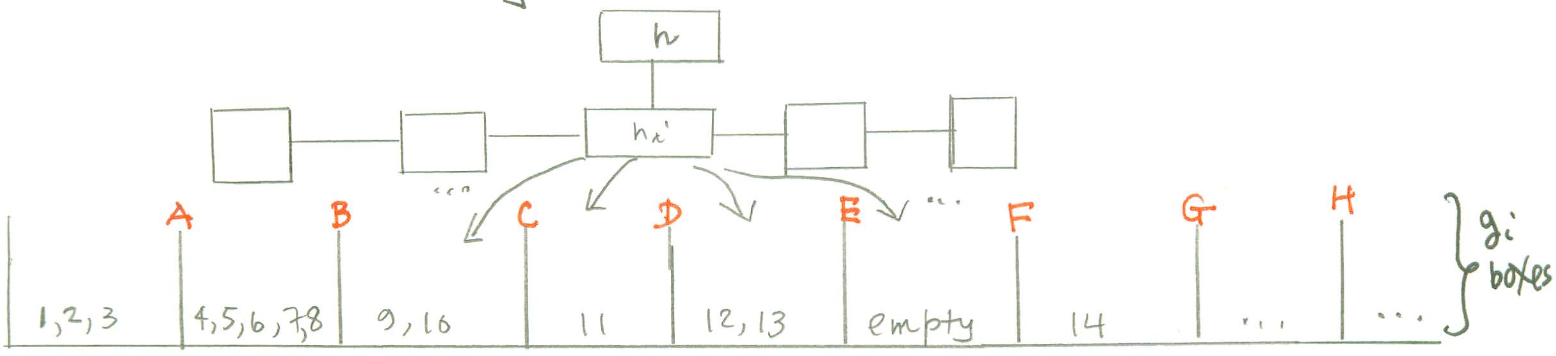
As in the M-B case the constraints are

$$\sum_i n_i = n \quad ; \quad \sum_i \epsilon_i n_i = E \qquad (1)$$

total energy

Let the degeneracy of each level be g_i; for example in hydrogen, for each value of the principal quantum number n there are $(2l+1)$ degenerate states (where l is the orbital angular momentum), each having the same energy. Hence even if we focus on a single energy state ϵ_i having n_i bosons, there is still a combinatoric question of how many ways can the n_i bosons be distributed among the g_i substates, all having the same energy ϵ_i?

This is where the major difference with fermions arises: for fermions each substate can have either $n_i = 0$ or $n_i = 1$ by virtue of the Pauli Exclusion Principle. Schematically:



As shown, one way to visualize the combinatoric problem is to number the particles and to then label the partitions A, B, C, ... Then a complete specification of this configuration would look like

$$\text{Config} = \quad 1,2,3, A\ 4,5,6,7,8, B \ldots \qquad (2)$$

By moving the partitions A, B, C, ... around they can end up in any position, which then allows each "box" to contain an arbitrary number of particles.

To obtain the total number of configurations as in (2) we begin by finding the number of permutations of $[n_i + (g_i - 1)]$ objects: n_i = number of particles, g_i = number of boxes (this requires $(g_i - 1)$ partitions since the ends are fixed). Hence the number of permutations is $[n_i + g_i - 1]!$

However, this treats the sequence of partitions A, B, C, ... and B, A, C, ... as physically different, which they are not, since the labels A, B, C, ... are artificial. Hence we must reduce the original number of permutations by the factor $(g_i - 1)!$

The original number of permutations also treats as distinct the case where the first bin has 1, 2, 3 and the j-th bin has 57, 93, 101, and the configuration where these are reversed. If we forget about the partitions (which we have first taken care of), then there are $n_i!$ equivalent ways of writing down the labels of the n_i particles. Hence we must reduce the number of permutations by $n_i!$ also. Hence altogether, the number of configurations possible for the energy state ϵ_i with degeneracy g_i is

$$\text{number of configurations}(\epsilon_i) = \frac{(n_i + g_i - 1)!}{(n_i)!\,(g_i - 1)!} \equiv \text{[redacted]} \binom{n_i + g_i - 1}{n_i} \tag{3}$$

Where Does the Boson Assumption Enter?

We do not impose any restrictions on n_i or g_i. In principle $g_i = 1$ for one i and zero otherwise, in which case all the particles n_i would be in the same state.

The expression in (3) gives the number of favorable configurations for a specific energy level ϵ_i with degeneracy g_i. Evidently, the total number of configurations, taking account of all ϵ_i is

$$G = \frac{(n_1+g_1-1)!}{n_1!\,(g_1-1)!} \times \frac{(n_2+g_2-1)!}{n_2!\,(g_2-1)!} \times \cdots \frac{(n_i+g_i-1)!}{n_i!\,(g_i-1)!} = \prod_i \frac{(n_i+g_i-1)!}{n_i!\,(g_i-1)!} \qquad (4)$$

We (again) invoke the basic statistical mechanics assumption that the <u>probability W of a given macroscopic being realized is proportional to the number G of microscopic states that correspond to that macroscopic state.</u>

$$W = (\text{Const})\, G \equiv C\,G \qquad (5)$$

For example, for the same number of particles n we could have a configuration with $n_1 = 1$ $(g_1 = 1)$ and $n_{17} = n-1$, with $g_{17} = 1$. This configuration would give

many such factors

$$G = \frac{(1+1-1)!}{1!\;0!} \times \left\{ \frac{0!}{0!\,0!} \cdots \frac{0!}{0!\,0!} \right\} \times \frac{((n-1)+1-1)!}{(n-1)!\;0!} \qquad (6)$$

$$= 1 \times \{1 \times 1 \times 1 \times \cdots\} \times \frac{(n-1)!}{(n-1)!\,0!} = 1 \qquad (7)$$

Hence there is only one microscopic configuration which can correspond to this set of conditions, and hence the corresponding macroscopic state is improbable. To find the most probable macroscopic state we proceed as in the M-B case to write

$$\ln W = \ln C + \sum_i \left\{ \ln(n_i+g_i-1)! - \ln(n!) - \ln(g_i-1)! \right\} \qquad (8)$$

We use <u>STIRLING's FORMULA</u> in the form:

$$\boxed{\ln(n!) \cong \ln(2\pi n)^{1/2} + n\ln n - n \cong n\ln n - n} \qquad (9)$$

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Assuming that $n_i >> 1$ and $g_i >> 1$ we have from (8) & (9)

$$\ln W \simeq \ln C + \sum_i \left\{ (n_i + g_i)\ln(n_i + g_i) - n_i \ln n_i - g_i \ln g_i \right\}$$

As before we introduce the Lagrange multipliers in the forms

$$\alpha\left(\sum_i n_i - n\right) = 0 \qquad \beta\left(\sum_i \epsilon_i n_i - E\right) = 0 \qquad (10)$$

Then form the function $F(n_i) = \ln W + (-\alpha)\left(\sum_i n_i - n\right) + (\beta)\left(\sum_i n_i \epsilon_i - E\right)$ (11)

$$F(n_i) = \underbrace{\ln C + (+\alpha n + \beta E)}_{\text{constants}} + \sum_i \left\{ (n_i + g_i)\ln(n_i + g_i) - n_i \ln n_i - g_i \ln g_i - \alpha n_i - \beta \epsilon_i n_i \right\} \qquad (12)$$

(The signs of α, β are arbitrary here)

To find the maximum of $F(n_i)$ — which gives the most probable configuration — we write:

CANCEL

$$\frac{\delta F(n_i)}{\delta n_0} = \cancel{(n_i + g_i)}\frac{1}{\cancel{n_i + g_i}} + \ln(n_i + g_i) - \cancel{n_i}\frac{1}{\cancel{n_i}} - \ln n_i - \alpha - \beta \epsilon_i = 0 \qquad (13)$$

$$-\delta F(n_i) = 0 = \left\{ \ln\left(\frac{n_i}{n_i + g_i}\right) + \alpha + \beta \epsilon_i \right\} \delta n_i \qquad (14)$$

these are linearly indep. once α, β are introduced

Hence $\ln\left(\frac{n_i + g_i}{n_i}\right) = \ln\left(\frac{g_i}{n_i} + 1\right) = \alpha + \beta \epsilon_i$ (15)

Exponentiating: $\frac{g_i}{n_i} + 1 = e^{\alpha + \beta \epsilon_i} \Rightarrow$

$$\boxed{n_i = \frac{g_i}{e^{\alpha + \beta \epsilon_i} - 1}} \qquad (16)$$

BOSE–EINSTEIN DISTRIBUTION

Comparison of Distribution Functions

<u>Maxwell-Boltzmann:</u> $\dfrac{g_i}{n_i} = e^{\alpha+\beta\epsilon_i} \longleftrightarrow n_i = \dfrac{g_i}{e^{\alpha+\beta\epsilon_i}}$

<u>Bose-Einstein:</u> $\dfrac{g_i}{n_i} + 1 = e^{\alpha+\beta\epsilon_i} \longleftrightarrow n_i = \dfrac{g_i}{e^{\alpha+\beta\epsilon_i} - 1}$

<u>Fermi-Dirac:</u> $\dfrac{g_i}{n_i} - 1 = e^{\alpha+\beta\epsilon_i} \longleftrightarrow n_i = \dfrac{g_i}{e^{\alpha+\beta\epsilon_i}+1}$

$$\rightarrow \frac{g_i}{e^{(\epsilon_i-\epsilon_F)k_BT}+1}$$

The connection among these results follows by noting that for a dilute gas (high temperature & low pressure) the number of available eigenstates g_i is large compared to the number of particles n_i. Then

$$\frac{g_i}{n_i} \pm 1 \cong \frac{g_i}{n_i} \Rightarrow \left\{\begin{matrix} B-E \\ F-D \end{matrix}\right\} \longrightarrow M-B$$

Hence all 3 distributions assume the form: $n_i = g_i e^{-\alpha} e^{-\beta\epsilon_i}$. But for the M-B distribution we can compare to the ideal gas laws etc. to find $\underline{\underline{\beta = 1/k_BT}}$. Hence this applies to the B-E and F-D distributions also.

LIMITS OF THE BINOMIAL DISTRIBUTION. I

THE GAUSSIAN DISTRIBUTION

Starting with the binomial distribution which is characterized by p and n we ask what happens in the limit as $n \to \infty$?

Consider many tosses of a die: Since the probability of getting any one number, say, [redacted] the number 1 is 1/6, the expected number of successes m is $m \cong (1/6)n$. This leads us to expect that the probability of getting m successes should peak near $m = pn$. To incorporate this we return to the binomial distribution

$$P(m) = p^m (1-p)^{n-m} \binom{n}{m} = p^m (1-p)^{n-m} \frac{n!}{m!\,(n-m)!} \qquad (1)$$

and use STIRLING's FORMULA*, for the case when both n and $m \approx pn$ are big.

[This distinguishes between the Gaussian and Poisson distributions: For Poisson, n is big but m remains small.]

$$* \quad n! \cong \sqrt{2\pi n}\; n^n e^{-n} \quad \Rightarrow$$

$$\binom{n}{m} = \frac{n!}{m!\,(n-m)!} \cong \frac{\sqrt{2\cancel{\pi} n}\; n^n \cancel{e^{-n}}}{\left(\sqrt{2\cancel{\pi} m}\; m^m \cancel{e^{-m}}\right)\left(\sqrt{2\pi(n-m)}\;(n-m)^{n-m}\cancel{e^{-(n-m)}}\right)} \qquad (2)$$

$$\overset{\text{algebra}}{=} \cdots\cdots = \frac{1}{\sqrt{2\pi n}} \left(\frac{m}{n}\right)^{-m-1/2} \left(\frac{n-m}{n}\right)^{-n+m-1/2} \qquad (3)$$

$$\boxed{\text{Hence:} \quad P(m) \cong \frac{1}{\sqrt{2\pi n}} \left(\frac{m}{n}\right)^{-m-1/2} \left(\frac{n-m}{n}\right)^{-n+m-1/2} p^m (1-p)^{n-m}} \qquad (4)$$

STIRLING FORMULA

We can rewrite Eq. (4) by using

$$y^x = \left(e^{\ln y}\right)^x = e^{x \ln y} \qquad (5)$$

$$\therefore\ P(m) = \frac{1}{\sqrt{2\pi n}} \exp\left\{ -\left(m+\tfrac{1}{2}\right)\ln\left(\frac{m}{n}\right) + \left(-n+m-\tfrac{1}{2}\right)\ln\left(\frac{n-m}{n}\right) + m\ln p + (n-m)\ln(1-p) \right\} \qquad (6)$$

Define $\boxed{m = np + \xi}$ ← ξ: deviation from the most probable value; np: most probable value of m ; $\xi \ll np$ is assumed

Then, after some algebra

$$P(m) \equiv P(\xi) = \frac{1}{\sqrt{2\pi n}} \exp\left\{ \overset{(1)}{-(np+\xi)\ln\left(1+\frac{\xi}{np}\right)} \overset{(2)}{-\frac{1}{2}\ln\left(p+\frac{\xi}{n}\right)} \overset{(3)}{-(n-np-\xi)\ln\left(1-\frac{\xi}{n-np}\right)} \underset{(4)}{-\frac{1}{2}\ln\left(1-p-\frac{\xi}{n}\right)} \right\} \qquad (7)$$

Up to this point the only approximation that has been made is the use of STIRLING's FORMULA for $n!$

To proceed we first drop the terms $\sim \xi/n$ in (2) and (4): This is safe to do because this leaves $\ln(p)$ or $\ln(1-p)$ which are non-zero. Hence collecting the remaining contributions:

$$(2)+(4) = e^{-\frac{1}{2}\ln p - \frac{1}{2}\ln(1-p)} = e^{-\frac{1}{2}\left[\ln p(1-p)\right]} = e^{\ln\left[p(1-p)\right]^{-1/2}} = \left[p(1-p)\right]^{-1/2} \qquad (8)$$

Hence up to this point:

$$P(\xi) \cong \frac{1}{\sqrt{2\pi np(1-p)}} \exp\left\{ -(np+\xi)\ln\left(1+\frac{\xi}{np}\right) - (n-np-\xi)\otimes \ln\left(1-\xi/n(1-p)\right) \right\} \qquad (9)$$

Even though $\xi \ll np$ is being assumed, we cannot invoke this approximation in the arguments of $\ln(\ldots)$ since this would leave $\ln(1)=0$. Rather, we must expand the $\ln(\ldots)$ using

$$\boxed{\ln(1+x) \cong x - \tfrac{1}{2}x^2 + \tfrac{1}{3}x^3 - \tfrac{1}{4}x^4 + \cdots} \qquad (10)$$

Hence in (9):

$$\{\ldots\} \cong -(np+\xi)\left(\frac{\xi}{np} - \frac{1}{2}\frac{\xi^2}{n^2p^2} + \cdots\right) - \left(n[1-p]-\xi\right)\left(\frac{-\xi}{n(1-p)} - \frac{1}{2}\frac{\xi^2}{n^2(1-p)^2} + \cdots\right) \quad (11)$$

$$= \cancel{-\xi} - \frac{\xi^2}{np} + \frac{1}{2}\frac{\xi^2}{np} + O(\xi^3) \cancel{+\xi} - \frac{\xi^2}{n(1-p)} + \frac{1}{2}\frac{\xi^2}{n(1-p)} + O(\xi^3) \quad (12)$$

key step!!

Hence $\{\ldots\} \cong -\frac{1}{2}\frac{\xi^2}{np} - \frac{1}{2}\frac{\xi^2}{n(1-p)} = -\frac{1}{2}\frac{\xi^2}{np(1-p)}$ (13)

It follows that $\boxed{P(m) \longrightarrow P(\xi) \cong \frac{1}{\sqrt{2\pi n(1-p)p}}\, e^{-(1/2)\,\xi^2/np(1-p)}}$ (14)

Define: $\sigma = \sqrt{np(1-p)} \Rightarrow$

$$\boxed{P(\xi) = \frac{1}{\sigma\sqrt{2\pi}}\, e^{-\xi^2/2\sigma^2}} \quad (15)$$

GAUSSIAN DISTRIBUTION

NOTES: ① This is the usual "Bell-Shaped Curve", where σ measures the width of the distribution

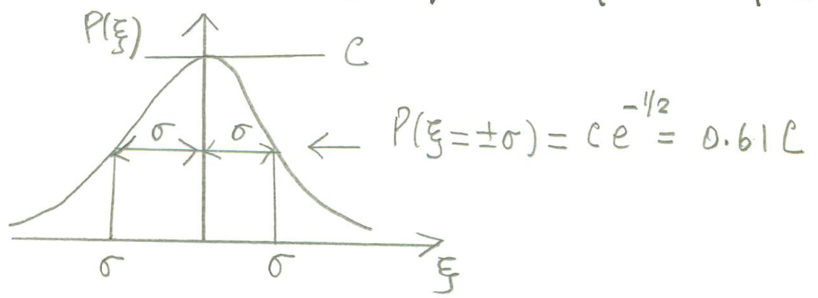
② The original dependence on m (# of successes) arises from the relation $\xi = m - np$.

③ Normalization: Recall that $\int_{-\infty}^{\infty} dy\, e^{-y^2/a^2} = a\sqrt{\pi}$ (16)

Here $a = \sigma\sqrt{2} \Rightarrow \frac{1}{\sigma\sqrt{2\pi}}\int_{-\infty}^{\infty} d\xi\, e^{-\xi^2/2\sigma^2} = 1$ ✓ (17)

④ Peak probability: $P(\xi)$ has a maximum at $\xi = 0 \Rightarrow m = np$ as expected.

$P(\xi=0) = 1/\sigma\sqrt{2\pi} \equiv C$.



LIMITS OF THE BINOMIAL DISTRIBUTION. II

THE POISSON DISTRIBUTION

As noted previously this is the case where the number of attempts $n \to \infty$, but where the number of successes $\boxed{m = np \equiv a}$ stays small.

As before we start with the BINOMIAL DISTRIBUTION

$$P(m) = p^m (1-p)^{n-m} \binom{n}{m} = p^m (1-p)^{n-m} \frac{n!}{m!\,(n-m)!} \qquad (1)$$

As before (Gaussian case) we use STIRLING's formula for $n!$ and $(n-m)!$, but NOT for $m!$ which remains small: $n! \cong \sqrt{2\pi n}\; n^n e^{-n}$ (2)

Hence,

$$\frac{n!}{(n-m)!} \cong \frac{n^{n+1/2}\, \cancel{e^{-n}}}{(n-m)^{n-m+1/2}\, e^{\cancel{-n}+m}} = \cdots = \frac{n^m e^{-m}}{(1-m/n)^{n-m+1/2}} \qquad (3)$$

Up to this point the only approximation has been the use of STIRLING's formula: We have not yet specified anything about the relative sizes of m and n. This comes next: In the denominator of (3) write

$$\left(1 - \frac{m}{n}\right)^{n-m+1/2} = e^{(n-m+1/2)\ln(1-m/n)} = e^{n(1-m/n+1/2n)\ln(1-m/n)} \qquad (4)$$

Now we invoke the assumption that the number of successes $m \ll n$:

Then we use $\ln(1+z) \cong z - \frac{1}{2}z^2 \cong z$ to write: $\ln(1-m/n) \cong -m/n$ (5)

Using (5), the r.h.s. of (4) can be written as

$$e^{\cancel{n}(1-m/n+1/2n)(-m/\cancel{n})} = e^{-m(1-m/n+1/2n)} \cong e^{-m} \qquad (6)$$

Hence altogether (1)–(6) $\Rightarrow$ $$\boxed{\frac{n!}{(n-m)!} \cong \frac{n^m \cancel{e^{-m}}}{\cancel{e^{-m}}} \cong n^m} \qquad (7)$$

The result in (7), which is very useful, can be verified as follows:

EXACT

$$\frac{n!}{(n-m)!} = \frac{n(n-1)(n-2)\cdots(n-[m-1])\cdot\cancel{(n-m)!}}{\cancel{(n-m)!}} = \underbrace{n(n-1)(n-2)\cdots(n-[m-1])}_{m\text{-factors}} \tag{8}$$

When $n \gg m \gg 1$ each surviving factor in (8) is $\simeq n$. Since there are m factors we recover (7):

$$n!/(n-m)! \cong n^m \tag{9}$$

As a further check on (7) & (9) we note that when $m=0$ both sides $= 1$ ✓

Combining (1) & (7) gives

$$P(m) = \frac{n!}{m!(n-m)!}\, p^m (1-p)^{n-m} \cong \frac{n^m}{m!}\, p^m (1-p)^{n-m} \tag{10}$$

Note that we do NOT use the STIRLING FORMULA here!

The p-dependent factors in (10) can be simplified as follows:

$$n^m p^m = (np)^m \equiv a^m = (\text{expected \# of successes})^m \tag{11}$$

Also: $$(1-p)^{n-m} = (1-p)^{a/p-m} \cong (1-p)^{a/p} = e^{a/p\,\ln(1-p)} \cong e^{(a/p)(-p)} = e^{-a} \tag{11'}$$

Recall: $p \ll 1$

Combining (10) – (11') we have

$$\boxed{P(m) \cong \frac{a^m e^{-a}}{m!} \; ; \; a = np = \text{expected \# of successes}} \tag{12}$$

POISSON DISTRIBUTION

This gives the probability of m successes in n tries when $p \ll 1$ for a single trial.

<u>NORMALIZATION:</u> $$\sum_{m=0}^{\infty} P(m) = e^{-a} \underbrace{\sum_{m=0}^{\infty} \frac{a^m}{m!}}_{e^a} = 1 \checkmark \tag{13}$$

Side Comment: In extending the sum on m to $m=\infty$ one may worry that the approximation $m \ll n$ may no longer hold. But for large m, the factor $1/m!$ suppresses the contributions from such terms, so that extending the sum to ∞ is compatible with the other approximations being made in arriving at (12).

Example: At each firing of a rifle the probability of achieving a hit on a target is 0.001. Find the probability of hitting a target with ≥ 2 bullets if the total number of shots fired $= 5000$.

Solution: Here $n = 5000$, $p = 0.001$, $a = np = 5$. $a \ll n$

$$\text{Then: } P(m) = \frac{5^m e^{-5}}{m!} \Rightarrow P(m \geq 2) = \sum_{m=2}^{\infty} \frac{5^m e^{-5}}{m!} \tag{14}$$

Hence, using the normalization condition in (13) we can write

$$P(m \geq 2) = \underbrace{\sum_{m=0}^{\infty} \left(\frac{5^m e^{-5}}{m!}\right)}_{1} - \left\{ P(m=0) + P(m=1) \right\} \tag{15}$$

$$P(m \geq 2) = 1 - \frac{5^0 e^{-5}}{0!} - \frac{5^1 e^{-5}}{1!} = 1 - 6\underbrace{e^{-5}}_{0.04043} = 0.9596 \tag{16}$$

Hence even though the probability for an individual success is small, the net probability for success is close to unity.

Comment: This example is based on experience during WW II.

COMMENTS ON GAUSSIAN & POISSON DISTRIBUTIONS

(1) Gaussian: Probability of success is relatively large e.g. toss of a die

Poisson: " " " " relatively small.

(2) For a Gaussian distribution the width $\sigma = \sqrt{np(1-p)}$. Note that as n increases the width increases: This makes sense, since the more times an experiment is repeated the more likely it is that a relatively improbable outcome will be realized. However, the relative width $\to 0$:

$$\text{relative width} \equiv \sigma/n = \sqrt{\frac{p(1-p)}{n}} \to 0$$