PHYS 353   Appendix

Probability and Distribution Functions

Part I. Binomial and Gaussian Distribution Functions

Notes: See the computer homework on volume 6: Radiation Statistics, the Introduction

Review: **Binomial Distribution**:   (discrete)

$$B(\#H) = [P^{\#H} * (1-P)^{\#notH} * N_c!] / [(\#H)! * (\#notH)!]$$

where (for the case of flipping a set of N_c coins):
   $B(\#H)$ = expected number of H's out of N_c individual events;
        (number of heads out of flipping N_c coins)

   P is the probability that H will appear in any given event;
        (in the case of honest coins, $P = 0.5$)

   (1 - P) is the probability that H will not appear in any given try;
        (in the case of honest coins, $P_{tails} = (1 - P_{heads}) = 0.5$, or the
         probability of tails)

   N_c is the number of individual events in any given try;
        (number of coins flipped in any one try)

   #H = number of H's (number of heads);

   #notH = number of not H's (number of tails).

Review: **Gaussian Distribution**   (continuous)

$$G(\#H) = \{1 / [2 \pi \sigma]\} \exp[-(\#H - AVG)/2\sigma^2]$$

where $AVG = Nc*P,$ $\sigma = \sqrt{[P * [1-P] * Nc]}$

IN-CLASS HOMEWORK: 3I-A
For 10 dice (or throwing one die 10 times), what is the probability that any particular number (say three) comes up
   a) 0 times?
   b) 1 time ?
   c) 2 times?
   d) do the Binomial Distribution results agree with the Gaussian?
   e) what is the sum of B(0)+ B(1) + ... + B(10) ?
   f) check your answers with the computer using computer homework: Advanced Physics, program
      Binomial.

HOMEWORK (3H-A):   do the problem section of Radiation Statistics

Notes: See the computer homework on volume 6: Half Life, the Introduction

HOMEWORK (3H-B):   do the problem section of Half Life

Part II. Boltzmann Distribution Function

Probability of one atom having n units of energy is based on equal likelihood of any state. Below is a listing of all possible states for two cases.

CASE I: four atoms having three units of energy:

	ABCD		ABCD	ABCD	ABCD	ABCD		ABCD
(3000) 4	3000	**(2100) 12**	2100	1200	1020	1002	**(1110) 4**	1110
	0300		2010	0210	0120	0102		1101
	0030		2001	0201	0021	0012		1011
	0003							0111

Prob of atom A having:
P(3) = 1/20 = .05
P(2) = 3/20 = .15
P(1) = 6/20 = .30
P(0) =10/20 = .50

CASE II: four atoms having five units of energy:

	ABCD		ABCD	ABCD	ABCD	ABCD		ABCD
(5000) 4	5000	**(4100) 12**	4100	1400	1040	1004	**(2111) 4**	2111
	0500		4010	0410	0140	0104		1211
	0050		4001	0401	0041	0014		1121
	0005							1112

	ABCD	ABCD	ABCD	ABCD		ABCD	ABCD	ABCD	ABCD
(3200) 12	3200	2300	2030	2003	**(3110) 12**	3110	1310	1130	1103
	3020	0320	0230	0203		3101	1301	1031	1013
	3002	0032	0032	0023		3011	0311	0131	0113

	ABCD	ABCD	ABCD	ABCD	ABCD	ABCD
(2210) 12	2210	2120	2102	1220	1202	1022
	2201	2021	2012	0221	0212	0122

Prob of atom A having:
P(5) = 1/56 = .018
P(4) = 3/56 = .054
P(3) = 6/56 = .107
P(2) =10/56 = .179
P(1) =15/56 = .268
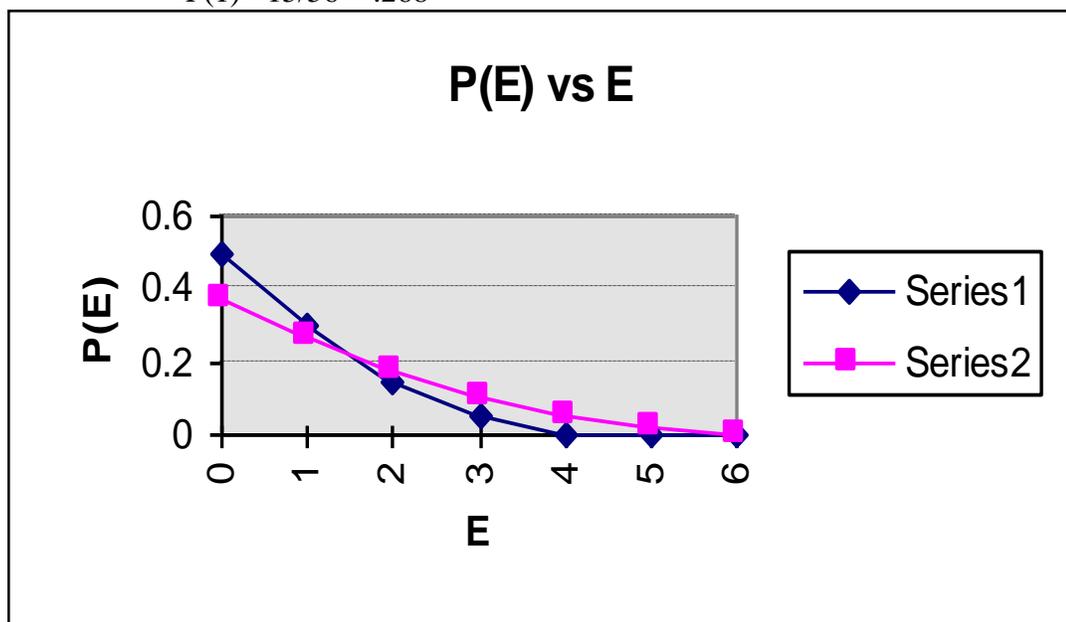
In general: $P(E) = A\,e^{-\alpha E}$ where A and α depend on the average energy, which depends on the temperature. For an average energy of kT (k being Boltzmann's constant $= 1.38 \times 10^{-23}$ Joules/Kelvin, $P(E) = A\,e^{-E/kT}$.

III.   Planck Distribution Function

a.   Energy of a phonon:
From the quantum theory, we know that for a harmonic oscillator, $[\hbar = h/2\pi]$
$E_{HO} = (n+\frac{1}{2})\hbar\omega$.   Since we are interested only in how the internal energy changes with Temperature, we can disregard the $\frac{1}{2}$.   Hence we can see that each phonon should have an energy of $hf = \hbar\omega$.

b.   Average number of phonons for any Temperature: (Planck distribution)
   b1)   Definition of average:
To find an average, we simply take the sum of the values and divide by the number of values.   Or we can take the sum of the values multiplied by their probability (and divide by the total probability which should be one).
   b2)   Probability of have n phonons: (Boltzmann distribution)
From probability theory we get that the probability of having a certain amount of something [here number of phonons] depends on how much of that something [total energy] there is and how many ways it can be divided [distributing the total energy among the total number of modes].   Assuming that each piece (each phonon) has an equal probability of belonging to any of the objects [modes], the probability of having a certain number of pieces [phonons] falls off exponentially.   This is the Boltzmann probability distribution.   For a more detailed example, see the previous page on the Boltzmann distribution.   The result is that the probability of having an energy, $E_n = n\varepsilon$, (here $\varepsilon = hw$, the energy of one phonon) is:

   $P(E_n) = A\,e^{-n\varepsilon/kT}$,   (Boltzmann distribution)
where k is Boltzmann's constant, T is the Temperature in Kelvins, and A is some amplitude such that the sum of all the probabilities is 1.

c)   Average number of phonons: (Planck distribution)
   From the basic definition of average, we have:

   $E_{avg}   =   n_{avg}\varepsilon   =   [\,_n\Sigma\,(n\varepsilon)\,A\,e^{-n\varepsilon/kT}\,] / [\,_n\Sigma\,A\,e^{-n\varepsilon/kT}\,]$;
we can divide through by ε, and we can divide out the A to get:
   $n_{avg}   =   [\,_n\Sigma\,n\,e^{-n\varepsilon/kT}\,] / [\,_n\Sigma\,e^{-n\varepsilon/kT}\,]$.
Here we become tricky.   Note that the numerator is the derivative of the denominator.   Recall that if we integrate dx/x we get the ln function.   So if we differentiate the ln function, we get dx/x.   From these facts:

   $-k\,T\,\partial\{\ln[\Sigma e^{-n\varepsilon/kT}]\}/\partial\varepsilon   =   [\,_n\Sigma\,n\,e^{-n\varepsilon/kT}\,] / [\,_n\Sigma\,e^{-n\varepsilon/kT}\,]   =   n_{avg}$.
Having experience with doing the Taylor series expansions forward, we can sometimes recognize an expansion as belonging to some function and effectively do the Taylor series expansion backwards:

   $_n\Sigma\,e^{-n\varepsilon/kT}   =   1 + e^{-\varepsilon/kT} + e^{-2\varepsilon/kT} + e^{-3\varepsilon/kT} + ...   =   1/[1 - e^{-\varepsilon/kT}]$.
Therefore, we can put this together to get:
   $n_{avg}   =   -k\,T\,d\{\ln[1/(1 - e^{-\varepsilon/kT})]\}/d\varepsilon   =   +k\,T\,d\{\ln[1 - e^{-\varepsilon/kT}]\}/d\varepsilon$
and now performing the differentiation:
   $n_{avg}   =   k\,T\,\{1/[1 - e^{-\varepsilon/kT}]\}\,\{0 - (-1/k_B T)\,e^{-\varepsilon/kT}\}   =   e^{-\varepsilon/kT}/[1 - e^{-\varepsilon/kT}]$
and multiplying through by $e^{+\varepsilon/kT}$:
   $n_{avg}   =   1/[e^{+\varepsilon/kT} - 1]$.   (Planck distribution)

IN-CLASS HOMEWORK :   3I-B
   a) Investigate n_{avg} for the low temperature limit ($\varepsilon \gg kT$);
   b) investigate n_{avg} for the high temperature limit ($\varepsilon \ll kT$).
   c) Is the Planck distribution a "classical" or a "quantum" distribution function?

   Before we proceed further, let's consider something called the **partition function**.   The idea behind the Boltzmann probability is that each possible arrangement is equally probable.   An important consideration, then, is going to be the number of possible states.
   By definition of average, the average energy, <E>, can be calculated as the value of each possible energy times the probability of having that energy, divided by the total probability of having any state (with $\beta = 1/kT$):

   $$<E> = \Sigma_r\{E_r \exp[-\beta E_r]\} / \Sigma_r\{\exp[-\beta E_r]\} .$$

We define the sum over all states as the partition function, Z:

   Z = $\Sigma_r\{\exp[-\beta E_r]\}$.   **Partition Function**

Further, note that the numerator in <E> is just:

   $$\Sigma_r \{E_r \exp[-\beta E_r]\} = \Sigma_r \{\partial(-\exp[-\beta E_r])/\partial\beta = -\partial Z/\partial\beta ;$$

Now recalling that $\partial \ln(y)/\partial x = (1/y) \, \partial y/\partial x$, we can write:

   $$<E> = -\partial(\ln[Z])/\partial\beta .$$

IV.   Quantum Distribution Functions

Special Case: two particles (A,B) in system with three states (1,2,3)

a) According to the classical theory (Maxwell-Boltzmann, or MB), each particle is distinguishable, and each state is distinguishable, so the possible ways of having the system are listed under the MB title at the top of the next page.

b) According to the Bose-Einstein statistics for particles with integer spin and symmetric wavefunctions, the particles are indistinguishable (due to the Heisenberg Uncertainty Principle) and more than one particle can be in any one state (due to + sign in the combination of wavefunctions).   The possible ways of having this are listed under the BE title.

c) According to the Fermi-Dirac statistics for particles with half-integer spin and anti-symmetric wavefunctions, the particles are indistinguishable and at most only one particle can be in any one state (due to - sign in the combination of wavefunctions).   The possible ways of having this one are listed under the FD title.

		MB			BE				FD		
States:	1	2	3		1	2	3		1	2	3
	AB	-	-		AA	-	-		A	A	-
	-	AB	-		-	AA	-		A	-	A
	-	-	AB		-	-	AA		-	A	A
	A	B	-		A	A	-				
	B	A	-		A	-	A			3 ways	
	A	-	B		-	A	A				
	B	-	A								
	-	A	B			6 ways					
	-	B	A								

9 ways

Define η as being equal to the probability of finding two particles in the same state divided by the probability of finding the two particles in different states. For the three cases above, we find that:

$$\eta_{MB} = 3/6 = 0.5; \quad \eta_{BE} = 3/3 = 1; \quad \eta_{FD} = 0/3 = 0.$$

(This seems to indicate that in the BE statistics, particles are MORE likely to be in the same state than classically, while they are prohibited from being in the same state in the FD statistics.)

HOMEWORK (3H-C):
        Perform the same analysis as above for two particles in four states, and calculate η for each of the three cases (MB, BE and FD).

We consider THREE CASES of quantum statistics PLUS the Maxwell-Boltzmann case. In each case we will calulcate an average number of particles in some state, s. To do this, we add up the number of particles in a state times the probability of the particle being in that state. We will use $<>$ to indicate average. We also use $\beta = kT$ for ease in writing.
        CASE 1: Bose-Einstein where the number of particles is not fixed (such as photons or phonons);
        CASE 2: Bose-Einstein where the number of particles IS fixed (such as alpha particles);
        CASE 3: Fermi-Dirac where the number of particles IS fixed (such as electrons).
        CASE 4: Maxwell-Boltzmann where the number of particles IS fixed and the particles are distinguishable!

CASE 1: BE with number of particles NOT fixed

$$<n_s> \;=\; \Sigma_{ns}\, n_s\, A\, exp[-\beta n_s \varepsilon_s] \,/\, \Sigma_{ns}\, A\, exp[-\beta n_s \varepsilon_s]$$

which says that the average number in state s is: {0 * probability of having 0 in state s} + {1 * probability of having 1 in state s} + etc. divided by the total probability of the system. Note that the A in the summations can come out of the summations since it is a constant, and so will cancel out of the expression. This is just the situation discussed for the Planck distribution!

$$\mathbf{n_{avg} \;=\; 1\,/\,[e^{+\varepsilon/kT} - 1]\,.} \qquad\qquad \mathbf{(Planck\ distribution)}$$

CASE 2: BE with number of particles FIXED

        In this case, if we have n_s in a state s, we must have $N - n_s$ particles in the other states. {Before, we were not tied to any particular number of particles, and so the number in state s did not affect the number in the other states. Therefore, the number in state s was simply related to the Boltzmann Probability of $A\, exp[-\beta n_s \varepsilon_s]$.} Here we must consider the probability of having n_s in state s AND the probability of having the others in the other states. This adds to the complexity of the expression above. Let's define the following:

$$N = \Sigma_r n_r\,; \quad N' \;=\; \Sigma_{r\ except\ s} n_r = N - n_s\,; \quad and$$

$$Z(N') \;=\; \Sigma_{n1,n2,...\ except\ ns} exp[-\beta(n_1\varepsilon_1 + n_2\varepsilon_2 + ...)]$$

where the sum for four particles (N=4) in four states (not a real example but one that we can at least follow) would look like, for $n_s = n_3 = 1$:

$$Z(N') \;=\; Z(N-n_s) \;=\; Z(4-1) \;=$$

$$\{\, exp[-\beta(3\varepsilon_1)] + exp[-\beta(2\varepsilon_1 + \varepsilon_2) + exp[-\beta(2\varepsilon_1 + \varepsilon_4)$$

$$+ exp[-\beta(\varepsilon_1 + 2\varepsilon_2)] + exp[-\beta(\varepsilon_1 + 2\varepsilon_4)] + exp[-\beta(\varepsilon_1 + \varepsilon_2 + \varepsilon_4)]$$

$$+ exp[-\beta(3\varepsilon_2)] + exp[-\beta(2\varepsilon_2 + \varepsilon_4)] + exp[-\beta(3\varepsilon_4)] \,\} \,.$$

Therefore, we can write for the average number of particles in state s:

$$\langle n_s \rangle \;=\; \{\Sigma_{n_s} n_s \exp[-\beta n_s \varepsilon_s]\, Z(N\text{-}n_s)\} \,/\, \{\Sigma_{n_s} \exp[-\beta n_s \varepsilon_s]\, Z(N\text{-}n_s)\}$$

$$= \;\frac{\{0 + \exp[-\beta\varepsilon_s]\, Z(N\text{-}1) + 2\exp[-2\beta\varepsilon_s]\, Z(N\text{-}2) + \ldots \}}{\{1 + \exp[-\beta\varepsilon_s]\, Z(N\text{-}1) + \exp[-2\beta\varepsilon_s]\, Z(N\text{-}2) + \ldots \}} \;.$$

IF $\delta N \ll N$, then by a Taylor series expansion we can write:

$$\ln[Z_s(N\text{-}\delta N)] \;\approx\; \ln[Z_s(N)] - (\partial\ln[Z_s(N)]/\partial N)\delta N = \ln[Z_s(N)] - \alpha_s \delta N$$

$$= \;\ln[Z_s(N)] - \alpha_s n_s \qquad \text{where} \qquad \alpha_s = \partial\ln[Z_s]/\partial N \approx \alpha$$

since the removal of only one state should affect Z very little.   Z should be very insensitive as to which n_s is removed, and so $\alpha_s \approx \alpha$.

Therefore, from the above equality:

$$\ln[Z_s(N\text{-}n_s)\} \;\approx\; \ln[Z_s(N)] - \alpha n_s \quad , \quad \text{or}$$

$$-\alpha n_s \;=\; \ln[Z_s(N\text{-}n_s)] - \ln[Z_s(N)] \;=\; \ln[Z_s(N\text{-}n_s)/Z_s(N)] \quad , \text{ or}$$

$$[Z_s(N\text{-}n_s)/Z_s(N)] \;=\; \exp[-\alpha n_s]\,.$$

We now use this in the above expression for $\langle n_s \rangle$:

$$\langle n_s \rangle \;=\; \frac{Z_s(N)\,\{0 + \exp[-\beta\varepsilon_s]\exp[-\alpha] + 2\exp[-2\beta\varepsilon_s]\exp[-2\alpha] + \ldots \}}{Z_s(N)\,\{1 + \exp[-\beta\varepsilon_s]\exp[-\alpha] + \exp[-2\beta\varepsilon_s]\exp[-2\alpha] + \ldots \}} \;.$$

or

$$\langle n_s \rangle \;=\; \Sigma_s n_s \exp[-n_s(\beta\varepsilon_s+\alpha)] \,/\, \Sigma_s \exp[-n_s(\beta\varepsilon_s+\alpha)] \;=\; 1\,/\,\{\exp[\beta\varepsilon_s+\alpha] - 1\}$$

where the last equality follows exactly the same derivation as the Planck derivation - the only difference is that the exponent is $\beta\varepsilon_s+\alpha$ instead of $\beta\varepsilon_s$.

Finally:

$\langle n_s \rangle \;=\; 1\,/\,\{\exp[\beta\varepsilon_s+\alpha] - 1\}.$ **Bose-Einstein Distribution**

The only difference between having a fixed number of particles (Bose-Einstein) and not (Planck) is the factor $\exp(\alpha)$.   The value of α can be calculated from:

$$N \;=\; \Sigma_r n_r \;=\; \Sigma_r(1\,/\,\{\exp[\beta\varepsilon_r+\alpha] - 1\}\,.$$

CASE 3:   FD with number of particles FIXED

For this case, n_s can only have the values 0 and 1!   Thus we have:

$$\langle n_s \rangle \;=\; \{0 + \exp[-\beta\varepsilon_s]\, Z_s(N\text{-}1)\} \,/\, \{Z_s + \exp[-\beta\varepsilon_s]\, Z_s(N\text{-}1)\}$$

$$= \; Z_s(N)\,\{0 + \exp[-\beta\varepsilon_s]\exp[-\alpha_s]\} \,/\, Z_s(N)\,\{1 + \exp[-\beta\varepsilon_s]\exp[-\alpha_s]\}$$

$$= \; \exp[-(\beta\varepsilon_s+\alpha)] \,/\, \{1 + \exp[-(\beta\varepsilon_s+\alpha)]\} \;=\; 1\,/\,\{\exp[\beta\varepsilon_s+\alpha] + 1\} \quad , \text{ so}$$

$\langle n_s \rangle \;=\; 1\,/\,\{\exp[\beta\varepsilon_s+\alpha] + 1\}\,.$ **Fermi-Dirac Distribution**

In Solid State Physics, we let $\alpha = -\beta\mu$, where μ is called the chemical potential.   When $\varepsilon = \mu$, $\langle n \rangle = \tfrac{1}{2}$.

CASE 4:   MB with the number of particles FIXED but the particles ARE distinguishable
 First consider the partition function, Z.   Since the particles ARE distinguishable, we must add the factor $N!/(n_1!n_2!...)$ to each expression in the Z function:

 $$Z(N) \;=\; \Sigma_{n1,n2,...}\{ [N!/(n_1!n_2!...)] \exp[-\beta(n_1\varepsilon_1+n_2\varepsilon_2+)] \}$$

 $$=\; \Sigma_{n1,n2,...}\{ [N!/(n_1!n_2!...)] \exp[-\beta n_1\varepsilon_1] \exp[-\beta n_2\varepsilon_2] ... \}$$

 $$=\; \Sigma_{n1,n2,...}\{ [N!/(n_1!n_2!...)] \exp[-\beta\varepsilon_1]^{\wedge}n_1 \exp[-\beta\varepsilon_2]^{\wedge}n_2 ... \}$$

but the above is just a binomial expansion, so:

 $$Z(N) \;=\; (\exp[-\beta\varepsilon_1] + \exp[-\beta\varepsilon_2] + ...)^{\wedge}N \; .$$

Further, we can write:

 $$\ln[Z] = N \ln\{\Sigma_r \exp[-\beta\varepsilon_r]\} \; .$$

Finally (using an expression similar to that for $<E_s> = -\partial[\ln(Z)]/\partial\beta$, but replace $\partial/\partial\beta$ with $(1/\beta)\partial/\partial\varepsilon_s$), we get:

 $$<n_s> \;=\; (-1/\beta)\,\partial[\ln(Z)]/\partial\varepsilon_s \;=\; (-1/\beta)\,N\,(-\beta\exp[-\beta\varepsilon_s])\,/\,\Sigma_r\{\exp(-\beta\varepsilon_r)\}$$

 $$=\; N \exp[-\beta\varepsilon_s]\,/\,\Sigma_r\{\exp[-\beta\varepsilon_r]\} \;=\; N * \text{Probability of being in state s;}$$

 $$<n_s> \;=\; N \exp[-\beta\varepsilon_s]\,/\,\Sigma_r\{\exp[-\beta\varepsilon_r]\} \quad , \quad \text{or}$$

 $$<n_s> \;=\; A \exp[-\beta\varepsilon_s] \;=\; 1\,/\,\{\exp[\alpha]\exp[\varepsilon/kT] \quad (\beta = 1/kT)\,, \quad \text{or}$$

 $$<n_s> \;=\; 1\,/\,\exp[\beta\varepsilon_s+\alpha] \; .\qquad\qquad \textbf{Maxwell Boltzmann Distribution}$$

<div align="center">COMPARISON OF THE THREE DISTRIBUTION FUNCTIONS</div>

 MB: $<n_s> \;=\; 1\,/\,\{\exp[\beta\varepsilon_s+\alpha]\}$

 BE: $<n_s> \;=\; 1\,/\,\{\exp[\beta\varepsilon_s+\alpha] - 1\}$ (Planck has $\alpha = 0$)

 FD: $<n_s> \;=\; 1\,/\,\{\exp[\beta\varepsilon_s+\alpha] + 1\}$

IF $\varepsilon \gg kT$, THEN BE & FD $\rightarrow$ MB, $n_{MB} \approx n_{FD} \approx n_{BE}$.

IF $\varepsilon \ll kT$, THEN $n_{BE} > n_{MB} > n_{FD}$.

IN-CLASS HOMEWORK: 3I-C

 a) For room temperature, find the range of frequencies for which MB $\approx$ BE.
 b) For the surface of the sun (T $\approx$ 6000 K), find the range of frequencies for which MB $\approx$ BE.
 c) For liquid helium temperatures (T $\approx$ 4 K), find the range of frequencies for which MB $\approx$ BE.
 d) Run the computer program entitled Quantum statistics from the Advanced Physics Menu.   Find values for α (and μ where $\alpha = -\beta\mu$) that give N = 50 for each case (in which there are 100 energy levels spaced .01 eV apart).   See if α and/or μ change with changing temperature.

HOMEWORK (3H-D):
 For the MB case of 4 particles: 2 in the first state, one in the second, zero in the third, and one in the fourth; list the possibilities and show that the number of possibilities is equal to $N!/[n_1! \, n_2! \, n_3! \, n_4!]$.

HOMEWORK (3H-E):
 Show that $\Sigma_{ns}\{\exp[-\beta n_s\varepsilon_s]\} = 1 + e^{-\beta\varepsilon s} + e^{-2\beta\varepsilon s} + ... \;=\; 1\,/\,[1 - e^{-\beta\varepsilon s}]$
by using a Taylor series expansion.   HINT: proceed backwards (that is, show that the result on the right equals the expression on the left).   HINT: let $x = \exp[-\beta\varepsilon_s]$.

Maxwell Velocity Distribution

Consider a molecule of mass m in a dilute gas.   Center of mass of the molecule is at **r**.
Momentum of center of mass of molecule is **p**.   If external forces such as gravity are neglected (usually a good approximation for fast moving dilute gases), then

$\qquad \varepsilon = p^2/2m + \varepsilon(\text{internal})$.

If the gas is dilute, the ε(internal) does NOT depend on **r**.   (We will treat the kinetic energy classically, which is a good approximation if the temperature is not too low.   The internal energies MUST be treated with quantum statistics.)

If we use the Maxwell-Boltzmann statistics: $\qquad\qquad$ Prob(**r,p**) $\propto$ exp[-β(p²/2m)] exp[-$\beta\varepsilon$(int)] d^3**r** d^3**p** .

The sum over all internal states causes the factor of exp[-$\beta\varepsilon$(int))] to just equal some constant.   Thus,

$\qquad$ Prob(**r,p**) $\propto$ exp[-β(p²/2m)] d^3**r** d^3**p** .

Now DEFINE the function, f, as:

$\qquad$ f(**r,v**) d^3**r** d^3**v** = the mean number of molecules with center of mass

position between **r** and r+**dr**, and velocity between **v** and **v+dv**.

$\qquad$ f(**r,v**) d^3**r** d^3**v** = C exp[-β(½mv²)] d^3**r** d^3**v**

where C is determined from normalization:

$\qquad$ f(**r,v**) d^3**r** d^3**v** = N = ∫ C exp[-β(½mv²)] d^3**r** d^3**v** = C V ∫exp[-β(½mv²)] d^3**v**

where the integral over space just gives the volume, V, since there is no spatial dependence in the probability function.

$\qquad$ Further, $\qquad$ ∫ exp[-β(½mv²)] d^3**v** = ∫∫∫ exp[-β(½m{v_x²+v_y²+v_z²})] dv_x dv_y dv_z

and since v_x, v_y and v_z are independent of one another, we can write the above as:

$\qquad$ = [∫ exp[-β(½mv_x²)] dv_x]³ = [2π/βm]$^{3/2}$.

Therefore, our normalization to get C gives:

$\qquad$ N = C V [2π/βm]$^{3/2}$,   or   C = (N/V) [βm/2π]$^{3/2}$ = nβ[βm/2π]$^{3/2}$

where   n = N/V   is the number density.   We now have for f:

$\qquad$ f(**v**) d^3**r** d^3**v** = n [m/2πkT]$^{3/2}$ exp[-mv²/2kT] d^3**r** d^3**v** .

To get the distribution of just the v_x speeds, we could integrate the above over all r and over v_y and v_z to get:

$\qquad$ $f_x(v_x)$ dv_x $\qquad$ = n [m/2πkT]$^{3/2}$ V (2πkT/m)$^{2/2}$ ∫exp[-mv_x²/2kT] dv_x

$\qquad\qquad\qquad\qquad$ = N [m/2πkT]$^{1/2}$ ∫exp[-mv_x²/2kT] dv_x .

The average v_x is:

$$\langle v_x \rangle = \int v_x f_x(v_x)\, dv_x = 0$$

since f_x is even and v_x is odd, and the integral is over $-\infty$ to $+\infty$.

However, if we evaluate $\langle v_x^2 \rangle$ we get:

$$\langle v_x^2 \rangle = \int v_x^2 f_x v_{(x)}\, dv_x \, / \int f_x(v_x)\, dv_x$$

$$= N\,[m/2\pi kT]^{1/2} \int v_x^2 \exp[-mv_x^2/2kT]\, dv_x \, / \, N = kT/m$$

so that $\frac{1}{2}m\langle v_x^2 \rangle = \frac{1}{2}kT$ (in agreement with the equipartition theorem.
For all three dimensions: $\langle v^2 \rangle = \langle v_x^2 + v_y^2 + v_z^2 \rangle = \langle v_x^2 \rangle + \langle v_y^2 \rangle + \langle v_z^2 \rangle$ so that
$\frac{1}{2}m\langle v^2 \rangle = \langle \frac{1}{2}mv^2 \rangle = (3/2)kT$. From this we can get:

$$v_{rms} = \sqrt{\langle v^2 \rangle} = \sqrt{[3kT/m]}$$

Let's now consider speed distributions: $F(v)\, dv =$ the mean number of

molecules per unit volume with a speed $v = |\mathbf{v}|$ in the range between v and v+dv.   To do this, we can convert from rectangular form (dv_x, dv_y, dv_z) to polar form: $(dv, v\, d\theta_v, v\sin(\theta)\, d\varphi_v)$ where the θ and φ dependence can be integrated out (no angular dependence in the integral) to give $4\pi v^2 dv$:

$$\mathbf{F(v)\, dv = f(v)4\pi v^2 dv = 4\pi n\,(m/2\pi kT)^{3/2}\, v^2 \exp[-mv^2/2kT]\, dv\,.}$$

This is the **Maxwell distribution of speeds**.

We can use this to get a mean speed and a most probable speed:

$$\langle v \rangle = (1/n)\,{}_0\!\int^\infty v\, F(v)\, dv = 4\pi\,(m/2\pi kT)^{3/2}\,{}_0\!\int^\infty v^3 \exp[-mv^2/2kT]\, dv = \sqrt{[8kT/\pi m]}$$

The most probable speed is when $F(v)$ is maximized:

$$v_{mp} \text{ is when } dF(v)/dv = 0 = d\{4\pi n(m/2\pi kT)^{3/2}v^2\exp[-mv^2/2kT]\}/dv\,.$$

Since the derivative is set equal to zero, we can cancel the constants:

$$v_{mp} \text{ is when } d\{v^2\exp[-mv^2/2kT]\}/dv = 0\,, \text{ or}$$

$$2v\exp[-mv^2/2kT] + v^2(-2mv/2kT)\exp[-mv^2/2kT] = 0,\text{ or}$$

cancelling out the common 2, v and $\exp[-mv^2/2kT]$ we get:

$$1 - mv^2/2kT = 0\,, \quad \text{or} \quad v_{mp} = \sqrt{[2kT/m]}\,.$$

Reviewing:

$$v_{mp} = \sqrt{[2kT/m]} = 1.000\,\sqrt{[2kT/m]}$$

$$\langle v \rangle = \sqrt{[(8/\pi)kT/m]} = 1.128\,\sqrt{[2kT/m]}$$

$$v_{rms} = \sqrt{[3kT/m]} = 1.224\,\sqrt{[2kT/m]}\,.$$

IN-CLASS HOMEWORK: 3I-D
        Find the v_{mp}, $\langle v \rangle$ and v_{rms} for N_2 molecules at room temperature, and run the computer program Maxwell from the Advanced Physics menu.