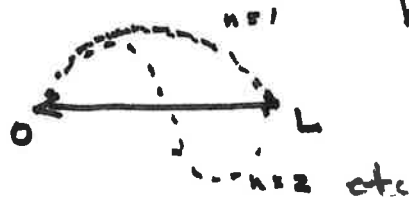


Problem 1: Counting states for gas particles in box

i) G+T 4.11

a 1-d box



$$k = \frac{\pi}{L} n$$

$$n = 1, 2, 3$$

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{n^2 \hbar^2}{8mL^2} \quad \text{G+T Eq (4.22)}$$

$$\text{So } n = \frac{2L}{\hbar} (2mE)^{1/2}$$

$$\text{So if we are given } E = 144 (\hbar^2/8mL^2)$$

$$\text{Then max } n \text{ is } n = \frac{2L}{\hbar} \frac{(2m)^{1/2} \hbar}{(8mL^2)^{1/2}} \cdot 12$$

$$n = 12 \text{ is \# of states } \ddot{\smile}$$

in book's language

$$I(E) = 12$$

ii) G+T 4.14

To estimate: # microstates for ^{single} gas in 1 liter box at Troom. Hint: Find $\tilde{E}$ from $\tilde{E} = \frac{3}{2} kT$.

Also: If energy interval is $\Delta E = 10^{-27} \text{ J} \dots$ which is lots smaller than $\tilde{E}$, find $g(E) \Delta E$, which is approximately the # microstates available to that molecule.

We will use 1-D # of total states energy $< E$

$$I(E) = \frac{4\pi V}{3 \hbar^3} (2mE)^{3/2}$$

$$\text{G+T Eq (4.42)}$$

$$\Rightarrow g(E) \Delta E \approx \frac{dI(E)}{dE} \Delta E = 2 \frac{5/2}{\hbar^3} \pi m^{3/2} E^{1/2} \Delta E$$

$$\text{G+T Eq (4.17)}$$

Numbers needed: let's say m is that of N_2 in Warmup prob 2 ... so $m = 4.6 \times 10^{-26} \text{ kg}$

Prob 1 (cont) $E = \frac{3}{2} kT$; $k = 1.38 \times 10^{-23} \text{ J/K}$
 $T = 300 \text{ K}$ (close enough)

Then $g(E) = \frac{2^{5/2} (1.001 \text{ m}^3)}{(6.64 \times 10^{-34} \text{ J}\cdot\text{s})^3} \cdot 3.14 \cdot (4.6 \times 10^{-26})^{3/2}$
 $(6.2 \times 10^{-21} \text{ J})^{1/2}$

And $\Delta E = 10^{-27} \text{ J}$

$\Rightarrow \underline{g(E) \Delta E = 5 \times 10^{22} \text{ states}}$

$kT = 4.14 \times 10^{-21}$
 single particle
 10^{22} states.

Problem 2

Entropy + The Einstein Solid: G+T Prob 4.7

Use "Entropy Einstein Solid" + explore entropies

(a) Try increasing $N_A, N_B + E_{\text{tot}} \dots$

- How do $S_A, S_B + S_{\text{tot}}$ depend on E_A ?
- Why does S_A increase with E_A while S_B decreases?
- Does S_{tot} have max at a certain E_A .

Before running code, can say
 $S_A \uparrow$ when $E_A \uparrow$ b/c $S(E)$ is monotonically increasing. Microscopically, more states $\leftrightarrow$ higher $E_A \leftrightarrow S_A = k \ln \Omega_A$ will grow. B/C $E_B = E_{\text{tot}} - E_A$, S_B must $\downarrow$ when $E_A \uparrow$.
 S_{tot} will be maximized when $E_A = \bar{E}_A$.

I will choose a couple of cases.

One $N_A = N_B = 50$ $E = 200$

Another $N_A = 20, N_B = 30$ $E = 200$

One: S_{tot} is maximized when $E_A = 100 = \bar{E}_A$

Another S_{tot} is maximized when $\bar{E}_A = 80 = E_A$

$$\bar{E}_B = 120$$

This is ratio of N_A/N_B .

(b) Notice how

One: $T_B \approx T_A \approx 2.47$ right at $E_A = \bar{E}_A$

Another: Again $T_B \approx T_A \approx 4.5$ right at $E_A = \bar{E}_A$

See picture below

Slopes are equal in mag
 (+ opposite in sign) when $\frac{1}{T_A} = \frac{1}{T_B}$
 Since $\frac{1}{T_i} = \frac{\partial S_i}{\partial E_i}$

Problem 1: G&T 4.7 : program EntropyEinsteinSolid:

One case (equal N_A and N_B) and Another case ($N_A < N_B$) shown below.



200
150
50

200
150
50

parameters and describe the qualitative behavior

next page



200
150
50

200
150
50

50 100

Also, see N dependence of relative error from only keeping max value of entropy:
 relative error in S : $S(\langle EA \rangle) / S$
 as last item in text below.

This program calculates the entropy of two Einstein solids that can exchange energy. The plot shows the entropy of the two systems, S_A (blue curve) and S_B (red curve), and the entropy S of the combined system, $S = S_A + S_B$, as a function of the energy E of system A. The total energy is given by $E = E_A + E_B$.

The entropy S is a function of the total energy E and the number of states Ω of the combined system. The entropy S_A of system A is given by

$$S_A = k_B \ln \Omega_A(E_A)$$

where $\Omega_A(E_A)$ is the number of states of system A with energy E_A . The entropy S_B of system B is given by

$$S_B = k_B \ln \Omega_B(E_B)$$

where $\Omega_B(E_B)$ is the number of states of system B with energy E_B .

$$S(E) = k_B \ln \left[\sum_{E_A} \Omega_A(E_A) \Omega_B(E - E_A) \right]$$

where E is the total energy of the combined system. The entropy S can be approximated by

$$S(E) \approx k_B \ln \left[\Omega_A(\hat{E}_A) \Omega_B(E - \hat{E}_A) \right]$$

NA	NB	$S(\langle EA \rangle) / S$
5	5	0.1439
50	50	0.0187
500	500	0.0056

As we'd expect, as N grows, this relative error decreases.

Problem 3 → Isolated Einstein Solid

G&T Problem 4.22

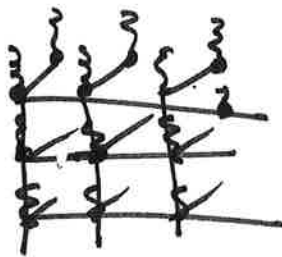
N disting. oses; total energy E .

Each is a 1-D oscillator, so

$$\epsilon_n = (n + \frac{1}{2})\hbar\omega$$

$$E = (Q + \frac{1}{2}N) \cdot \hbar\omega$$

with Q total # of quanta



Want to calculate $T(E)$, dependence of Temp on E in μ canon ensemble.

$$\text{Use } \Omega = \frac{(Q + N - 1)!}{Q! (N - 1)!}$$

Let us rewrite Ω using $Q = \frac{E}{\hbar\omega} - N/2$

$$\Rightarrow \Omega = \left[\frac{E}{\hbar\omega} + \frac{N}{2} - 1 \right]!$$

$$\left[\frac{E}{\hbar\omega} - \frac{N}{2} \right]! [N - 1]!$$

$$S = k \ln \Omega$$

• Stirling's approx
• ignore "1" next to $N/2$

$$\begin{aligned} \frac{S}{k} &= \left(\frac{E}{\hbar\omega} + \frac{N}{2} \right) \ln \left(\frac{E}{\hbar\omega} + \frac{N}{2} \right) - \left(\frac{E}{\hbar\omega} + \frac{N}{2} \right) \\ &\quad - \left(\frac{E}{\hbar\omega} - \frac{N}{2} \right) \ln \left(\frac{E}{\hbar\omega} - \frac{N}{2} \right) + \left(\frac{E}{\hbar\omega} - \frac{N}{2} \right) \\ &\quad - N \ln N + N \end{aligned}$$

$$\text{And } \frac{1}{T} = \frac{\partial S}{\partial E} = \frac{k}{\hbar\omega} \left[\ln \left(\frac{E}{\hbar\omega} + \frac{N}{2} \right) - \ln \left(\frac{E}{\hbar\omega} - \frac{N}{2} \right) \right]$$

$$\frac{1}{T} = \frac{k}{\hbar\omega} \ln \frac{E/\hbar\omega + N/2}{E/\hbar\omega - N/2}$$

Problem 3 (cont)

$$\text{Thus } T = \frac{\hbar\omega}{k} \left[\ln \frac{E/\hbar\omega + N/2}{E/\hbar\omega - N/2} \right]^{-1}$$

Now invert for $E(T)$

$$e^{\frac{\hbar\omega}{kT}} = \frac{E/\hbar\omega + N/2}{E/\hbar\omega - N/2}$$

$$\Rightarrow (E/\hbar\omega - N/2) e^{\frac{\hbar\omega}{kT}} = E/\hbar\omega + N/2$$

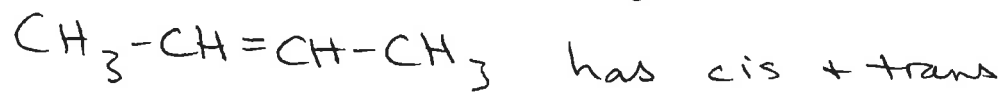
$$\Rightarrow E = \frac{N\hbar\omega}{2} \frac{(e^{\hbar\omega/kT} + 1)}{(e^{\hbar\omega/kT} - 1)}$$

$$= N\hbar\omega \left(\frac{1}{2} + \frac{1}{e^{\hbar\omega/kT} - 1} \right)$$

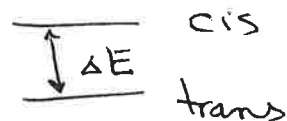
$$\text{so } E = \frac{N\hbar\omega}{2} + \frac{N\hbar\omega}{e^{\hbar\omega/kT} - 1}$$

Problem 4

G+T 4.24 This hydrocarbon, 2-butene



isomers, $\frac{\Delta E}{k} = 4180 \text{ K}$



What is relative abundance at $T=300\text{K} + T=1000\text{K}$

Answer: $\frac{P_{\text{cis}}}{P_{\text{trans}}} = e^{-\frac{\Delta E}{kT}}$

Ratio is

$T=300\text{K}$

$e^{-\frac{4180}{300}} \approx 8.9 \times 10^{-7}$

$T=1000\text{K}$

$e^{-\frac{4180}{1000}} \approx 1.5 \times 10^{-2}$

Problem 5 - Maximizing the Shannon Entropy

B+B 15.3

Want to maximize $S = -k \sum_i P_i \ln P_i$ Let $\alpha, \beta \equiv 1 \dots$ would change optimization problem

subject to $\sum_i P_i = 1$

$$\langle f(x) \rangle = \sum_i P_i f(x_i)$$

↑ some constant...

We will use Method of Lagrange Multiplier

$$S = - \sum_i P_i \ln P_i - \alpha \sum_i P_i - \beta \sum_i P_i f(x_i)$$

$\langle f(x) \rangle$ is confusing... let's call it f_0

$$S = - \sum_i P_i \ln P_i - \alpha \sum_i P_i - \beta \sum_i P_i f(x_i)$$

$$dS = 0 \Rightarrow \frac{\partial S}{\partial P_j} = 0 \quad \text{for any } P_j$$

$$\Rightarrow -\ln P_j - 1 - \alpha - \beta f(x_j) = 0$$

$$\Rightarrow P_j = e^{-(1+\alpha) - \beta f(x_j)}$$

Then $\sum_i P_i = 1 = e^{-(1+\alpha)} \sum_i e^{-\beta f(x_i)}$

So if $Z(\beta) = \sum_i e^{-\beta f(x_i)} = e^{+(1+\alpha)}$

Then $P_j = \frac{1}{Z(\beta)} e^{-\beta f(x_j)}$

and then $\langle f_0 \rangle = \sum_i f(x_i) P_i$

$$= \frac{1}{Z} \left(- \frac{\partial}{\partial \beta} Z \right) = - \frac{\partial \ln Z}{\partial \beta}$$

Problem 6

Semiclassical limit of ideal Gases

1) G+T Problem 6.2

To show: Volume dep. of Z_1 is indep. of box shape. eg. Eq. (6.10):

$$Z_1 = V \left(\frac{2\pi m}{\beta h^2} \right)^{3/2}$$

Should be derivable if $V = L_x L_y L_z$

NB $\lambda = \frac{h}{\sqrt{2\pi m kT}}$ so $Z_1 = \frac{V}{\lambda^3}$ wow!

$$\epsilon_{n_x, n_y, n_z} = \frac{\hbar^2 \pi^2}{2m} \left[\left(\frac{n_x}{L_x} \right)^2 + \left(\frac{n_y}{L_y} \right)^2 + \left(\frac{n_z}{L_z} \right)^2 \right]$$

is generalization of Eq. 6.3

$$\text{Thus } Z_1 = \sum_{n_x, n_y, n_z} e^{-\beta \frac{\hbar^2 \pi^2}{2m} \left[\left(\frac{n_x}{L_x} \right)^2 + \left(\frac{n_y}{L_y} \right)^2 + \left(\frac{n_z}{L_z} \right)^2 \right]}$$

$$\therefore Z_1 = S_x S_y S_z$$

(6.9)

$$= L_x \left(\frac{2\pi m}{\beta h^2} \right)^{1/2} \quad \text{sim}$$

$$\therefore Z_1 = L_x L_y L_z \left(\frac{2\pi m}{\beta h^2} \right)^{3/2} \quad \checkmark$$

Problem 6 (cont)

$\bar{\lambda}$ for N_2 at T_{room} ?

$$\bar{\lambda} = \frac{h}{\sqrt{2\pi m k T}}$$

$$T_{\text{room}} = 298 \text{ K}$$

$$\Rightarrow 1.91 \times 10^{-11} \text{ m}$$

So $\rho = \frac{N}{V}$ so when volume per N was around $\bar{\lambda}^3$...

$$V = \bar{\lambda}^3 = 6.94 \times 10^{-33} \text{ m}^3/\text{molecule}$$

$$\Rightarrow \frac{N}{V} = 1.44 \times 10^{32} \frac{\text{molecules}}{\text{m}^3} = 1.44 \times 10^{26} \frac{\text{molecules}}{\text{cm}^3}$$

If say $P = P_{\text{atm}} = 10^5 \text{ N/m}^2$

use $P = \frac{N}{V} k T$ just to start

$$\Rightarrow T = \frac{P}{\frac{N}{V} k} = 0.00005 \text{ K}$$

Clearly, ideal gas eqn doesn't hold!

N_2 is solid, polly.

Check web for density of solid N_2
 0.25 g/cm^3 . We have $1.44 \times 10^{26} \text{ molecules/cm}^3$

Real
This is
much denser
than the
classical
solid,
 N_2

Problem 6 : (cont)

1 mole weighs 28 g so

0.25 g/cm³ would be about
 $\frac{1}{100}$ mole or 6×10^{21} molecules/cm³

So solid N₂ is much less dense
(a classical solid!) than this
condensate.

Problem 7 G&T Prob 6.9

Entropy of Mixing

(a) Explain (6.40) in simple terms:

This is $\Delta S = 2Nk \ln 2$ if $N_A = N_B = N$
 $V_A = V_B = V$

This result suggests that

New - Old entropy per particle
is $k \ln 2$.

Since $S = k \ln \Omega$, This is

$$\ln \Omega_{\text{new}} - \ln \Omega_{\text{old}} = 2$$

$$\frac{\Omega_{\text{new}}}{\Omega_{\text{old}}} = 2 \quad \text{which makes sense.}$$

Particle has double the volume, so,
looking back either at $\Sigma_i \propto V$
or at $I(E) \propto V$, volume
has doubled

(b) If we had used

$$\text{Eq. (6.31)} \quad S = Nk [\ln V + f(T, m)] \quad \text{Non-identical form for } \Sigma W$$

$$\text{We'd get } S_{\text{new}} = 2Nk \ln 2V + 2Nk f(T, m)$$

But Eq. (6.27) yields

$$S_{\text{new}} = 2Nk \ln \frac{2V}{2N} + 2Nk f(T, m)$$

Prob 7
cont

So using former rather than latter we'd get
for identical particles

$$\Delta S = 2Nk \ln 2V - 2Nk \ln V$$

$$= 2Nk \ln 2$$

~~for identical particles~~

Problem 8 → Equipartition

(i) B&B 19.5 If $E = \alpha x^2$

$$dE = \alpha dx$$

$$dx = \frac{1}{\alpha} dE$$

$$\Rightarrow \langle E \rangle = \frac{\int_0^\infty E e^{-\beta E} dx}{\int_0^\infty e^{-\beta E} dx} = \frac{\frac{1}{\alpha} \int_0^\infty E e^{-\beta E} dE}{\frac{1}{\alpha} \int_0^\infty e^{-\beta E} dE} = \frac{1}{\beta} = \underline{\underline{kT}}$$

(There is option for demon theorem.
problem to let $E \sim p \sim \text{got}$)

$$E_d = \frac{1}{3} \langle \frac{E}{N} \rangle = \frac{1}{3} \cdot \underset{\substack{\uparrow \\ 3D}}{3} kT = kT \checkmark$$

(ii) G&T 6.47

... (see Figure 6.5). It is a good approximation to take the rotational and vibrational motion to be independent and to express the total energy of an ideal diatomic gas as a sum of the translational, rotational, and vibrational contributions. Hence the total heat capacity (at constant volume) of the gas can be written as

$$C = C_{\text{tran}} + C_{\text{rot}} + C_{\text{vib}}. \quad (6.257)$$

The last two terms in (6.257) arise from the internal motion of the molecule. The rotational contribution C_{rot} was discussed in Problem 6.46.

Problem 8 cont

- (a) The vibrational motion of a diatomic molecule can be modeled by harmonic oscillations about the minimum of the potential energy of interaction between the two molecules. What is the high temperature limit of C_{vib} ?

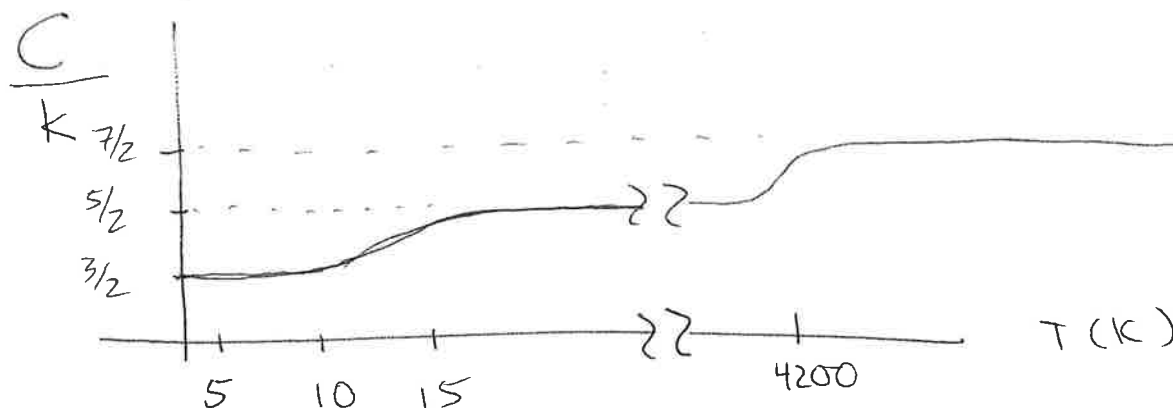
Solution. There are two quadratic contributions to the vibrational energy, the kinetic energy and the spring-like potential energy. Thus, for each molecule the contribution to C_{vib} is k .

- (b) Let us define a temperature $T_{vib} = \hbar\omega/k$. The magnitude of T_{vib} for HCl is $T_{vib} \approx 4227$ K, where ω is the vibrational frequency and $\hbar\omega$ is the energy difference between neighboring vibrational energy levels. What do you expect the value of C_{vib} to be at room temperature?

Solution. At room temperature, which is much less than T_{vib} , we expect the vibrational states of the molecules to not be excited, and thus $C_{vib} \approx 0$.

- (c) Use the value of T_{rot} given in Problem 6.46 and the value of T_{vib} given in part (b) for HCl to sketch the T -dependence of the total heat capacity C in the range $10 \text{ K} \leq T \leq 10000 \text{ K}$.

Solution. There are three plateaus of $(3/2)k$, $(5/2)k$, and $(7/2)k$ and smooth curves connecting them near $T = T_{rot} = 15$ K, for the transition between purely translation contributions to the specific heat to contributions from both translational and rotational contributions, and then near $T = T_{vib} = 4227$ K at which vibrational contributions become important.



Problem 9 → M-B veloc Dist G+T Prob 6.11

- (a) Program LJ2DFluidMD simulates a system of particles interacting via the Lennard-Jones potential (1.1) in two dimensions by solving Newton's equations of motion numerically. The program computes the distribution of velocities in the x -direction among other quantities. Compare the form of the velocity distribution to the form of the Maxwell velocity distribution in (6.60). How does its width depend on the temperature?

Solution. Some typical data for $N = 64$, $L = 20$, with $\Delta t = 0.01$ and various initial kinetic energies per particle are summarized in Table S6.1. The runs were equilibrated for 10^4 time steps and averaged over about 3×10^4 time steps. Figure S6.1 shows that the width is proportional to $T^{1/2}$. The temperature was estimated from the equipartition theorem and is not simply related to the initial kinetic energy.

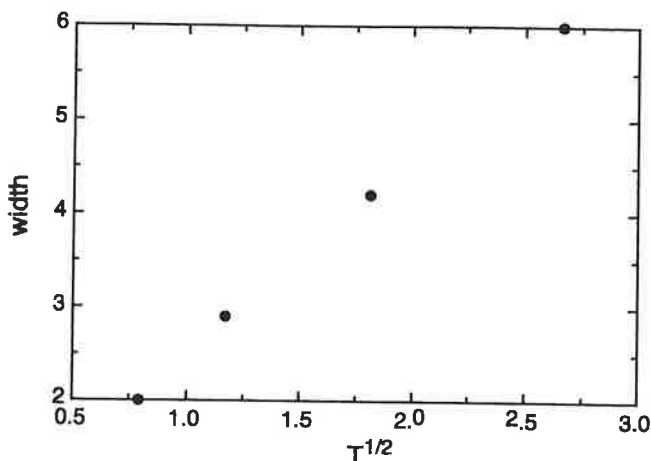
initial kinetic energy	T	width
0.01	0.63	2.0
1.00	1.37	2.9
3.00	3.28	4.2
5.00	7.09	6.0

Table S6.1: Data from Program LJ2DFluidMD. The width (full width at half maximum) is obtained from a Gaussian fit to the histogram of the velocities in the x direction.

- (b) Program TemperatureMeasurementIdealGas implements the demon algorithm for an ideal classical gas in one dimension (see Section 4.9). All the particles have the same initial velocity. The program computes the distribution of velocities among other quantities. What is the form of the velocity distribution? Give an argument based on the central limit theorem (see Section 3.7) why the distribution has the observed form. Is this form consistent with (6.60)?

Solution. The velocity distribution can be fit to a Gaussian. This result can be understood from the central limit theorem, because the velocity of each particle is the sum of many random changes due to energy exchanges with the demon.

(b) Eq (6.60) is $f(v_x) = \left(\frac{m}{2\pi kT}\right)^{1/2} e^{-mv_x^2/2kT}$



Plot of the width in Table S6.1 as a function of $T^{1/2}$.

Problem 10

G + T Prob 6.12

Problem 6.12. Maxwell speed distribution.

- (a) Compare the form of the Maxwell speed distribution (6.61) with the form of the Maxwell velocity distribution (6.59).

Solution. The velocity distribution for any component v_i is symmetric about $v_i = 0$. The speed distribution is defined only for $v \geq 0$ and is not symmetric about any value of v .

- (b) Use the normalization condition $\int_0^\infty f(v) dv = 1$ to calculate A and show that

$$f(v) dv = 4\pi v^2 \left(\frac{m}{2\pi kT} \right)^{3/2} e^{-mv^2/2kT} dv. \quad (\text{Maxwell speed distribution}) \quad (6.62)$$

Solution. We start with

$$f(v) dv = 4\pi A v^2 e^{-mv^2/2kT} dv. \quad (6.61)$$

The normalization condition is

$$\int_0^\infty f(v) dv = 1, \quad (\text{S6.21})$$

which gives $4\pi A I_2/2 = 1$, where [see (A.17)]

$$I_2 = \int_{-\infty}^\infty x^2 e^{-ax^2} dx = \frac{1}{2} \left(\frac{\pi}{a^3} \right)^{1/2} \quad (\text{S6.22})$$

with $a = m/2kT$. Thus,

$$\pi A \left(\frac{\pi}{(m/2kT)^3} \right)^{1/2} = A \left(\frac{\pi}{(m/2kT)} \right)^{3/2} = A \left(\frac{2\pi kT}{m} \right)^{3/2} = 1, \quad (\text{S6.23})$$

and

$$A = \left(\frac{m}{2\pi kT} \right)^{3/2}. \quad (\text{S6.24})$$

- (c) Calculate the mean speed $\bar{v}$, the most probable speed $\tilde{v}$, and the root-mean square speed v_{rms} and discuss their relative magnitudes.

Prob 10 (cont)

Solution. The mean speed $\bar{v}$ is given by

$$\bar{v} = \int_0^{\infty} v f(v) dv = 4\pi A I_3, \quad (\text{S6.25})$$

where from (A.26),

$$I_3 = \int_0^{\infty} x^3 e^{-ax^2} dx = -\frac{\partial I_1}{\partial a} = -\frac{\partial}{\partial a} \frac{1}{2a} = \frac{1}{2a^2}. \quad (\text{S6.26})$$

Hence,

$$\bar{v} = 4\pi \left(\frac{m}{2\pi kT} \right)^{3/2} \frac{1}{2(m/2kT)^2} = 2 \left(\frac{2kT}{\pi m} \right)^{1/2}. \quad (\text{S6.27})$$

We obtain the most probable speed by taking the derivative of $f(v)$ and setting the result equal to 0:

$$(2\bar{v} - \bar{v}^2)(m\bar{v}/kT) = 0, \quad (\text{S6.28})$$

or

$$\bar{v} = \left(\frac{2kT}{m} \right)^{1/2}. \quad (\text{S6.29})$$

To find v_{rms} we first find the mean of v^2 given by $\bar{v^2} = 4\pi A I_4/2$, where

$$I_4 \equiv \int_{-\infty}^{\infty} x^4 e^{-ax^2} dx = -\frac{\partial I_2}{\partial a} = -\frac{\partial}{\partial a} \left[\frac{1}{2} \left(\frac{\pi}{a^3} \right)^{1/2} \right] = \frac{3}{4} \left(\frac{\pi}{a^5} \right)^{1/2}. \quad (\text{S6.30})$$

Thus,

$$\bar{v^2} = 2\pi \left(\frac{m}{2\pi kT} \right)^{3/2} \frac{3}{4} \left(\frac{\pi}{(m/2kT)^5} \right)^{1/2} = \frac{3kT}{m}. \quad (\text{S6.31})$$

This result is consistent with the equipartition theorem which gives $m\bar{v^2}/2 = 3kT/2$. Thus,

$$v_{\text{rms}} = \sqrt{\bar{v^2}} = \left(\frac{3kT}{m} \right)^{1/2}. \quad (\text{S6.32})$$

The three speeds depend on kT/m in the same way and are related by $v_{\text{rms}} = (3/2)^{1/2} \bar{v} \approx 1.22\bar{v}$ and $\bar{v} = (4/\pi)^{1/2} \tilde{v} \approx 1.13\tilde{v}$; v_{rms} and $\bar{v}$ are greater than $\tilde{v}$ because of the long tail in the speed distribution.

(d) Make the change of variables $u = v/\sqrt{(2kT/m)}$ and show that

$$f(v)dv = f(u)du = (4/\sqrt{\pi})u^2 e^{-u^2} du, \quad (\text{6.63})$$

where we have again used same the same notation for two different, but physically related probability densities. The (dimensionless) speed probability density $f(u)$ is shown in Figure 6.2.

Solution. Because $v = u\sqrt{(2kT/m)}$, we have

$$f(u)du = 4\pi(u\sqrt{(2kT/m)})^2 \left(\frac{m}{2\pi kT} \right)^{3/2} e^{-m[u\sqrt{(2kT/m)}]^2/2kT} d(u\sqrt{(2kT/m)}) \quad (\text{S6.33a})$$

$$= \frac{4}{\sqrt{\pi}} u^2 e^{-u^2} du. \quad (\text{S6.33b})$$

Optional
Problem

Monty hall Problem via Bayesian Stats

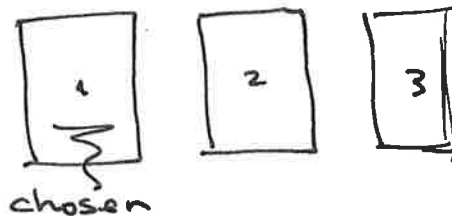
Event A_i : car is behind door i

Event B_i : host opens door i

Definition: $P(E)$ means probability of event E
 $P(E|E_g)$ means probability that
given E_g occurs, E occurs

Known Contestant chooses one of 3 doors
w.l.o.g. call it door 1

Host opens a door, call it j



Now, contestant would like

know $P(A_1|B_j)$... likelihood car is
behind chosen door, given host opened door j .

Calculations: Host's mentality is known...
host knows where car is!

$$P(B_2|A_1) = \frac{1}{2}$$

$$P(B_2|A_2) = 0$$

$$P(B_2|A_3) = 1$$

could also calculate $P(B_3|A_i)$ but these would
be quite similar... $P(B_3|A_1) = \frac{1}{2}$; $P(B_3|A_2) = 1$; $P(B_3|A_3) = 0$

$$P(A_1) = P(A_2) = P(A_3) = \frac{1}{3}$$

$$P(B_1) = 0$$

$$P(B_2) = \sum_i P(B_2 | A_i) P(A_i)$$

$$P(B_2) = \frac{1}{2} \cdot \frac{1}{3} + 0 \cdot \frac{1}{3} + 1 \cdot \frac{1}{3} = \frac{1}{2}$$

$$P(B_3) = \frac{1}{2}$$

Ready to use Bayes' Theorem:

eg. $P(A_1 | B_2) = \frac{P(B_2 | A_1) P(A_1)}{P(B_2)}$

stick $\curvearrowright$ given host opens door 2 $\curvearrowright$

$$= \frac{\frac{1}{2} \cdot \frac{1}{3}}{\frac{1}{2}} = \frac{1}{3}$$

also $P(A_1 | B_3) = \frac{P(B_3 | A_1) P(A_1)}{P(B_3)} = \frac{1}{3}$

No matter whether host opens door 2 or 3, Prob of (sticking) + winning is $\frac{1}{3}$

Checking what we expect ...

if switch to door 3 $\curvearrowright$

$$P(A_3 | B_2) = \frac{P(B_2 | A_3) P(A_3)}{P(B_2)}$$

$$= \frac{1 \cdot \frac{1}{3}}{\frac{1}{2}} = \frac{2}{3}$$

also if switch to door 2 $\curvearrowright$

Prob of (switching + winning) $\frac{2}{3}$

$$P(A_2 | B_3) = \frac{P(B_3 | A_2) P(A_2)}{P(B_3)}$$

$$= \frac{1 \cdot \frac{1}{3}}{\frac{1}{2}} = \frac{2}{3}$$

G+T 3.25

Accuracy refers to how many true positives and true negatives a test delivers.

$$A = P(+ | \text{ill}) \quad \text{true positive}$$

and also $A = P(- | \text{well}) \quad \text{true negative}$

Life doesn't have to be this way! A test could have different probs of true pos + true neg. But we are told to assume these are same.

It is true from probability theory that

$$P(+ | \text{ill}) + P(- | \text{ill}) = 1$$

$$\therefore P(- | \text{ill}) = 1 - A$$

An ill person must get some result

Similarly

$$P(+ | \text{well}) + P(- | \text{well}) = 1$$

$$\therefore P(+ | \text{well}) = 1 - A$$

What a person wants to know is

$$P(\text{ill} | +)$$

Bayes' Theorem:

$$P(\text{ill} | +) = \frac{P(+ | \text{ill}) P(\text{ill})}{P(+)}$$

where $P(+)$ = $P(+ | \text{ill}) P(\text{ill}) + P(+ | \text{well}) P(\text{well})$

Thus,

$$P(\text{ill} | +) = \frac{A P(\text{ill})}{A P(\text{ill}) + (1-A)(1-P(\text{ill}))};$$

This is $P(\text{well})$

Let $P(\text{ill}) = \epsilon$

Then $P(\text{ill} | +) = \frac{A \epsilon}{A \epsilon + 1 - A - \epsilon + A \epsilon}$

so $P(\text{ill} | +) = \frac{A \epsilon}{2A \epsilon + 1 - A - \epsilon} \quad (1)$

Suppose $P(\text{ill} | +) = 0.50$

$\epsilon = 0.01 \Rightarrow 0.50 = \frac{0.01}{0.02 + \frac{0.99}{A}} - 1$

$\Rightarrow \underline{A = 0.99 \dots 99\%}$

Suppose $P(\text{ill} | +) = 0.50$; $\epsilon = 0.001$

$\Rightarrow A = 0.999 \dots 99.9\%$

In general

Given $P(\text{ill} | +) = 0.50 = \frac{1}{2}$

* Can solve Eq. (1) & get

$A = 1 - \epsilon$