Problem 1. Energy In Combustion

Note: This is one of the few places where one needs to work rather precisely to see the physics point. My rule of thumb is that an Avagadros number times an electron volt is 100 kJ. But, here should use a more accurate evaluation, $N_A \cdot \mathrm{eV} = 96.5\,\mathrm{kJ}$. In evaluating the numbers below you should keep to an accuracy of one part in a thousand, $R = 8.314\,\mathrm{J/K{\cdot}mol}$.

(a) (Optional) Repeat the argument presented in class for the equation

$$dH = đQ_{\rm in} + V\,dp \tag{1}$$

where $H = U + pV$ represents the enthalpy. Enthalpy is particularly useful when the pressure is constant, leading to

$$dH = đQ_{\rm in} \tag{2}$$

(b) Consider the combustion of Hydrogen gas:

$$\mathrm{H}_2(g) + \frac{1}{2}\mathrm{O}_2(g) \leftrightarrow \mathrm{H}_2\mathrm{O}(l)\,. \tag{3}$$

resulting in the formation of liquid water vapor. Tables of enthalpies for reactions are available in many books.

(i) Look up the enthalpy of the products and reactants at 298 °K and standard pressure[1] in the accompanying data table. Determine the change in enthalpy, ΔH°, for each mole of H_2O produced.

(ii) Consider the reactants as ideal gasses, and treat the liquid product H_2O as having negligible volume compared to the gasses. Calculate the heat released during the combustion and the change in internal energy, $\Delta U^{\circ} = U_{\rm final} - U_{\rm initial}$, per mole. (Ans: $Q_{\rm out} = 285.8\,\mathrm{kJ}$ and $\Delta U = -282.1\,\mathrm{kJ}$)

(c) Consider the reaction at

$$\mathrm{H}(g) + \mathrm{H}(g) \rightarrow \mathrm{H}_2(g) \tag{4}$$

at NTP, which is accompanied by a large release of heat. Using the enthalpy data tables, determine the energy of a bond between the two atoms in a H_2 molecule in eV. (Ans: $\Delta U = -433.5\,\mathrm{kJ}$ and $\Delta = 4.48\,\mathrm{eV}$.)

Hint: First use the enthalpy data tables to determine the enthalpy change and heat released during the reaction. Use this to find ΔU for the reaction, treating all components as ideal gasses. The energy of a single H_2 molecule is its kinetic energy (translational and rotational) and its potential (or binding) energies:

$$E_{\mathrm{H}_2} = \mathrm{KE} + \mathrm{PE} = \mathrm{KE} - \Delta \tag{5}$$

[1] This temperature and pressure is the so-called Normal Temperature and Pressure (NTP) and denoted with a circle, i.e. T°, p° and H° denote the temperature, pressure, and enthalpy at NTP.

Here PE $= -\Delta$ is the binding energy (i.e. the bond energy) of the two atoms. (The negative sign indicates that the energy is lower when the two atoms are bound compared to when they are unbound. Δ is a positive value and is what we are trying to find.) The total energy U is the sum of kinetic and potential energies of the atoms. Use what we know about the kinetic energy of ideal gasses (both the mono-atomic and diatomic cases) to relate ΔU for one mol of H_2 produced to Δ.

Combustion

$\boxed{a)}$ See lecture

$\boxed{b)}$ Looking in the tables $\Delta_f H$ for H_2O is $H_1 = -285.8$ kJ per mole, while H_2 an O_2 have $\Delta_f H = 0$. So

$$\Delta H = -285.8 \text{ kJ} < 0$$

Now $\Delta H = Q_{in}$ at constant pressure so

$$\boxed{Q_{out} = 285.8 \text{ kJ}}$$

☆ To determine ΔU we need the work

$$\Delta U = Q_{in} - W_{out}$$

$$= Q_{in} - P_0 \big(\overset{0 \text{ Small}}{\cancel{V_{H_2O}}} - V_{H_2} - V_{\frac{1}{2} H_2O} \big)$$

Now

$$pV = n_{ml} RT \quad \text{so} \quad n_{ml} = \tfrac{1}{2} \text{ for } O_2 \text{ and}$$

thus

$$-W_{out} = \underbrace{RT}_{\text{from } H_2} + \underbrace{\tfrac{1}{2} RT}_{\text{from } O_2} = \frac{3}{2} RT \simeq (1.5)(8.32 \tfrac{J}{°k})(298°k)$$

$$= 3.7 \text{ kJ}$$

So

$$\Delta U = Q_{in} - W_{out} = -285.8\,kJ + 3.7\,kJ$$

$$\boxed{\Delta U = -282.1\,kJ}$$

note the work is small compared to heat, here.

c) Then using the data tables

$$\Delta H = -436\ kJ = Q_{in}$$

this is for 1 mol of H_2

The explanation was given in the tables.

Now

$$\Delta U = Q_{in} - p_o(V_{H_2} - 2V_{H_2})$$

So $pV = n_{m} RT$ so

again this is small

$$-W_{out} = \underbrace{-RT}_{1\,mol\ H_2} + \underbrace{2RT}_{2\,mol\ H} = RT = 2.47\,kJ$$

So

$$\boxed{\Delta U = Q_{in} - W_{out} = -436\ kJ + 2.5\,kJ = -433.5\,kJ}$$

Now

$$\Delta U = KE_f + PE_f - (KE_i + \cancelto{0}{PE_i})$$

$$= \underbrace{\frac{5}{2} N_A kT}_{\text{one mole of diatomic gas}} + PE_f - \underbrace{2\,\frac{3}{2} N_A kT}_{\text{2 moles of monoatomic gas}}$$

$$= -\frac{1}{2} RT + PE_{final}$$

or $$PE_{final} = \Delta U + \frac{1}{2} RT = -433\ kJ + 1.2\ kJ = -432.3\ kJ$$

This is for one mole of H_2. Using $N_A eV = 96.5\ kJ$

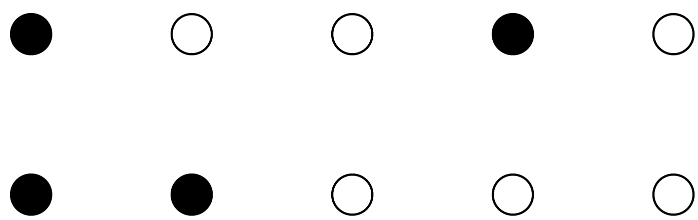
$$\boxed{PE_f = -N_A \Delta = -432.3\ kJ \qquad \Delta = 4.48\ eV}$$

Problem 2. Combinatorics and The Stirling Approximation

(a) Consider one mole of atoms laid out in a row. The atoms can be in two states, a ground state, and an excited state. 1/3 of them are in the excited states. Using the Stirling approximation, show that the number of configurations with this number of excited states is approximately

$$\Omega = 10^{1.67\times 10^{23}} \tag{6}$$

For instance, if the number of atoms is five, and the number of excited atoms (shown by the black circles) is 2, then two possible configurations are shown below.



(b) Now repeat the calculation, but work with symbols rather than numbers. Assume there are N atoms laid out in a row. Assume that N_1 of them are in the ground state, and N_2 are in the excited state, with $N_1 + N_2 = N$. Show that the log of the number of configurations is

$$\ln\Omega = -\sum_{i=1,2} N_i \ln(N_i/N) \tag{7}$$

$$= N\sum_{i=1,2} -P_i \ln P_i \tag{8}$$

In the last step we have recognized that the $P_1 = N_1/N$ is the probability that an atom will be in the ground state, and $P_2 = N_2/N$ is the probability that an atom will be in the excited state.

Discussion: The log of the number of configurations $\ln\Omega$ is known as the entropy of the system[2]. Then entropy per site, i.e. $\ln\Omega/N$, is given by

$$\frac{\ln\Omega}{N} = \sum_i -P_i \ln P_i \tag{9}$$

which is known as the Shannon formula for the entropy of a probability distribution. The importance of these things will become clearer as the course progresses.

[2] Actually $\ln\Omega$ is the entropy up to a conventional constant. For historical reasons the entropy is defined as $k_B \ln\Omega$, with k_B the Boltzmann constant. Similarly the entropy per site is defined only up to a conventional constant and later in the course we will respect tradition and take $-k_B\sum_i P_i \ln P_i$ as the entropy per site.

Combinatorics and Stirling

- The number of selections is

$$^{N_A}C_r = \frac{N_A!}{\left(\frac{1}{3}N_A\right)!\left(\frac{2}{3}N_A\right)!} \qquad \text{with } r \equiv \frac{1}{3}N_A$$

- Taking the log

$$\log {}^{N_A}C_r = \log N_A! - \log\left(\left(\tfrac{1}{3}N_A\right)!\right) - \log\left(\left(\tfrac{2}{3}N_A\right)!\right)$$

$$= N_A \log N_A - N_A - \left(\frac{1}{3}N_A \log\left(\frac{1}{3}N_A\right) - \frac{1}{3}N_A\right)$$

$$- \left(\frac{2}{3}N_A \log\left(\frac{2}{3}N_A\right) - \frac{2}{3}N_A\right)$$

$$= \frac{1}{3}N_A \log(3) + \frac{2}{3}N_A \log\left(\frac{3}{2}\right)$$

$$= \frac{N_A}{3}\log\left(\frac{27}{4}\right) = 0.64\,N_A$$

- So

$$^{N_A}C_r = e^{0.64 N_A} = \left(e^{\log 10}\right)^{0.64 N_A/\log 10}$$

$$= 10^{0.64 N_A/\log 10} \simeq 10^{1.66\times 10^{23}}$$

Combinatorics Continued:

$$\Omega = \frac{N!}{N_1!\,N_2!}$$

So

$$\ln \Omega = \ln N! - \sum_{i=1,2} \ln N_i!$$

Then using sterling $\ln N! = N \ln N - N$

$$\ln \Omega = N \ln N - \cancel{N} - \sum_i N_i \ln N_i - \cancel{N_i}$$

use $N = \sum N_i$ use $N = \sum N_i$

So

$$\ln \Omega = \sum_i N_i (\ln N - \ln N_i)$$

$$\boxed{\ln \Omega = \sum_i -N_i \ln N_i / N}$$

or pulling out N and with $P_i = N_i / N$

$$\boxed{\ln \Omega = N \sum_i -P_i \ln P_i}$$

Problem 3. Parametrizing the EOS

The pressure as a function of temperature an volume, $p(T, V)$, or equivalently the volume as a function of temperature and pressure $V(T, p)$, is an important physical observable. Recall that its changes are parameterized by the measurables β_p and κ_T. Similarly

Consider an ideal gas at temperature T with N particles

(a) Explain the physical meaning of the thermal expansion coefficient β_p and isothermal compressibility κ_T, and compute them for an ideal gas.

The first items only involved the EOS, $p(T, V)$. The next items also involves the energetics $U(T, V)$, so the specific heat and adiabatic index play a role. Assume that $U = c_0 T$ with c_0 a constant

(b) Write down c_0 for mono-atomic and diatomic ideal gasses, the specific heats C_p and C_v for these gasses, and the adiabatic index γ for these gasses.

(c) For for a general substance (and not necessarily an ideal gas) the specific heats C_p and C_V are are related by a formula which we will prove in full generality only later:

$$C_p = C_V + \frac{VT\beta_p^2}{\kappa_T}\,. \tag{10}$$

For an ideal gas we proved the following special case of this formula:

$$C_p = C_V + Nk_B\,. \tag{11}$$

Or, for one mole of substance

$$C_p^{1\text{ml}} = C_V^{1\text{ml}} + R\,. \tag{12}$$

Show that Eq. (12) follows from Eq. (10) together with the results from parts (a).

(d) The *adiabatic* compressibility κ_S is the defined by[3]

$$\kappa_S \equiv \frac{-1}{V}\left(\frac{\partial V}{\partial p}\right)_{adiab} \tag{14}$$

This "*adiab*" means that as we change the pressure, the volume and temperature change, so that no heat flows, $đQ = 0$. Show for an ideal gas that

$$\kappa_S = \frac{\kappa_T}{\gamma} \tag{15}$$

We will show later that this result is not limited to an ideal gas.

[3]The suffix S means adiabatic, $đQ = 0$. We will see that $đQ$ is related to the change in entropy S, $\mathrm{d}S = đQ/T$. So S suffix means at fixed entropy.

$$\kappa_S \equiv \frac{-1}{V}\left(\frac{\partial V}{\partial p}\right)_S \equiv \frac{-1}{V}\left(\frac{\partial V}{\partial p}\right)_{adiab} \tag{13}$$

(e) As discussed in class, the speed of sound is related to the compressibility[4]

$$c_s = \sqrt{\frac{B_S}{\rho}} \tag{16}$$

where the bulk modulus

$$B_S \equiv -V \left(\frac{\partial p}{\partial_V}\right)_{adiab} \equiv \frac{1}{\kappa_S} \tag{17}$$

serves as a kind of spring constant for the material, and ρ is the mass per volume. Air is made of diatomic molecules, primarily (78%) diatomic nitrogen N_2. Determine the speed of sound of N_2 gas at 20^oC treating using only the ideal gas constant R and the fact that a nitrogen atom consists of 7 protons and 7 neutrons. Compare with the nominal value for the speed of sound in air. You should find favorable agreement.

(f) The frequency of the tuning note ($A440$) in the orchestra is 440 Hz. Explain qualitatively why it is the adiabatic compressibility κ_S, and not the isothermal one κ_T which is relevant for the speed of sound, by comparing the time scales of oscillation with a typical time scale for heat conduction. Consider the following questions. When you turn on the heat on a frying pan, how long does it take to get hot? How does this time scale compare to the time it takes for sound to propagate across several meters.

[4] I will not derive this. A good derivation at your level is given here. Unfortunately, this derivation uses the symbol κ for B_S, which for us (and indeed almost everyone) is $1/\kappa_S$!

Parametrizing the EOS

a) For the meaning see lecture. I explained them as well as I could there! Now $V = NkT/p$

$$\beta_p = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_p = \frac{1}{V}\left(\frac{\partial}{\partial T}\right)_p \cdot \left(\frac{NkT}{p}\right) = \frac{Nk}{p}\frac{1}{V} = \frac{1}{T}$$

$$K_T = -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_T = \frac{-1}{V}\left(\frac{\partial}{\partial T}\right)_T \frac{NkT}{p} = \frac{1}{\left(\frac{NkT}{p}\right)}\left(+\frac{NkT}{p^2}\right) = \frac{1}{p}$$

b) Then

$$\boxed{\begin{array}{ll} U = \frac{3}{2}NkT & \text{MAIG} \\ U = \frac{5}{2}NkT & \text{DAIG} \end{array}}$$

c) $C_V = \left(\frac{\partial U}{\partial T}\right)_V = \frac{3}{2}Nk$ MAIG

$C_V = \left(\frac{\partial U}{\partial T}\right)_V = \frac{5}{2}Nk$ DAIG

$C_p = C_V + Nk$ All ideal gasses

$C_p = \frac{5}{2}Nk$ MAIG

$C_p = \frac{7}{2}Nk$ DAIG

So

$$\gamma = C_p / C_v = \frac{5}{2} \Big/ \frac{3}{2} = \frac{5}{3} \qquad \text{MAIG}$$

$$\gamma = C_p / C_v = \frac{7}{2} \Big/ \frac{5}{2} = \frac{7}{5} \qquad \text{DAIG}$$

$\boxed{d)}$ $$C_p = C_v + TV \frac{\beta_p^2}{\kappa_T}$$

Now $V = \frac{NkT}{p}$ $\quad \beta_p = \frac{1}{T}$ $\quad \kappa_T = \frac{1}{p}$

So

$$C_p = C_v + T \left(\frac{NkT}{p}\right) \frac{p}{T^2}$$

$$C_p = C_v + Nk$$

$\boxed{e)}$ C_p is larger than C_v because for the same change in temperature, dT, you must add more heat; since some of the thermal energy is being used for mechanical work as the gas expands to keep the pressure constant

Basically in a solid or liqued the coefficient β_p is small. Does a solid expand by much when you heat it? In a gas the system expands alot when heated.

Compare

$\beta_p \simeq 1 \times 10^{-4}\ {}^\circ K^{-1}$ mercury ← this is one of the liquids with the largest β_p !

$\beta_p \simeq 3 \times 10^{-3}\ {}^\circ K^{-1}$ gas

β_p gas $\simeq 30\ \beta_p$ mercury

$\boxed{f)}$ We have for an adiabatic expansion $Q = 0$

$$pV^{\gamma} = \text{const}$$

So

$$V^{\gamma}\, dp + p\gamma V^{\gamma - 1}\, dV = 0$$

$$dp + \gamma \frac{p}{V}\, dV = 0$$

So we find

$$-\frac{1}{V}\left(\frac{dV}{dp}\right)_{\text{adiab}} = \frac{1}{p\gamma}$$

We had for an ideal gas we had from (a)

$$\frac{1}{p} = \kappa_T$$

So

$$\kappa_S = \frac{\kappa_T}{\gamma}$$

In air we have

78 % N_2
22% O_2 ← We will neglect O_2 and consider N_2 gas.

So

$$C_s = \left(\frac{B_s}{\rho}\right)^{1/2} = \left(\frac{1}{K_s \rho}\right)^{1/2} = \left(\frac{\gamma}{K_T \rho}\right)^{1/2}$$

$$= \left(\frac{\gamma p}{\rho}\right)^{1/2} = \left(\frac{\gamma \cancel{N} kT}{V\rho}\right)^{1/2} \qquad V\rho = mN$$

$$c_s = \left(\frac{\gamma kT}{m}\right)^{1/2} \qquad \gamma = \frac{7}{5} \leftarrow \text{Diatomic!}$$

$m = 28\, m_p$ ← N_2 has 28 nucleons

So

A nucleon is either a proton or a neutron.

$$C_s = \left(\frac{\gamma \; N_A k \; T}{28 \; N_A m_p}\right)^{1/2}$$

$$C_s = \left(\frac{\gamma}{28} \frac{RT}{1g}\right)^{1/2} = \left(\frac{7/5 \;\; 8.32\, J/K \;\; 293°K}{28 \;\; 0.001 kg}\right)^{1/2}$$

$$\boxed{C_s = 349 \text{ m/s}}$$

For comparison in O_2 gas we have

$C_s \simeq 327$ m/s

Problem 4. Probability

In a short computer program, I produced 1000 random numbers generated uniformly between $[0, 1]$. I made a histogram[5] of these numbers which is shown in Fig. 1(a). (Histograms can be made with excel, google sheets, Mathematica, python, . . .) The first seven random numbers produced by the program are shown in the first column of the table below. For each random number I applied two functions $y_1(x) = 1/x$ and $y_2(x) = -\log(x)$, which are shown in the second and third columns respectively. I made histograms of y_1 and y_2 and these are shown in Fig. 1(b) and (c).

x	$y_1 = 1/x$	$y_2 = -\log(x)$	$y_3(x) =?$
0.536581	1.86365	0.622537	0.812603
0.895263	1.11699	0.110638	0.963793
0.0470624	21.2484	3.05628	0.361042
0.537013	1.86215	0.621732	0.812821
0.752013	1.32976	0.285002	0.909372
0.80406	1.24369	0.218081	0.929886
0.382136	2.61687	0.961978	0.725670
. . .	. . .	. . .	. . .

(a) Check the second and third column in the first row of the table shown above.

(b) Explicitly find three continuous functions which approximately describes the histograms in Fig. 1 (a), (b) and (c). The first function is a only a function of x, the second is a only a function y_1, and the third is a only a function only of y_2. Explain both the shape and the magnitudes of your function. I have drawn the functions I am looking for on top of the histograms. How are your functions related to the probability densities $P(y_1) \equiv \mathrm{d}\mathscr{P}/\mathrm{d}y_1$ and $P(y_2) \equiv \mathrm{d}\mathscr{P}/\mathrm{d}y_2$?

Hint: You can check your work by plotting your functions and see if they look like those shown in the figure, agreeing both in shape and in magnitude.

(c) Given a random number generator producing uniform numbers between 0 and 1, how could you produce random numbers with probability distribution $\mathrm{d}\mathscr{P}_y = 3y^2\mathrm{d}y$ with $y \in [0, 1]$?

Hint: Try to come up with a map $y(x)$ so that $P(x)\mathrm{d}x = \mathrm{d}x$. I applied this map to each x_i, denoted $y_3(x)$, recording the results in the fourth column of the table given above. You can check that you have the right map by checking the numbers in this column. A histogram of y indeed produces the right distribution, Fig. 1(d).

[5] Wikipedia provides a quick review of histograms. Briefly a histogram counts the number of events or outcomes (i.e. rows in the table of this problem) with x_i between x and $x + \Delta x$. The bin width is Δx.

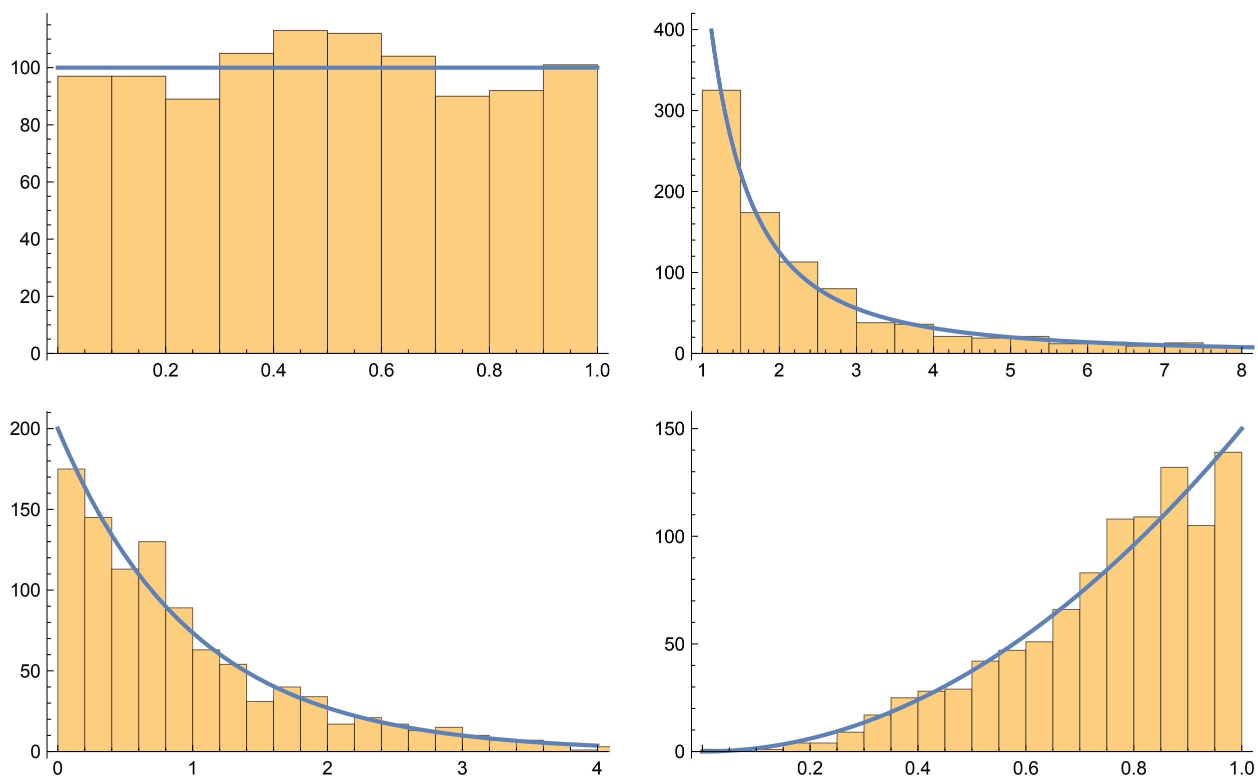


Figure 1: **Top Row (a) and (b):** Histogram of x and y_1. **Bottom Row (c) and (d):** Histogram of y_2 and y_3

Solution:

(a)

(b) We have $P(x) = 1$

$$\mathrm{d}\mathscr{P} = P(x(y))|\frac{dx}{dy}|dy \tag{18}$$

We have $x(y_1) = 1/y_1$ and $x(y_2) = \exp(-y_2)$. The derivatives are

$$\left|\frac{dx}{dy}\right| = \frac{1}{y_1^2} \qquad \left|\frac{dx}{dy}\right| = \exp(-y_2) \tag{19}$$

So in the two cases we have

$$\frac{\mathrm{d}\mathscr{P}}{dy_1} = \frac{1}{y_1^2} \qquad \frac{\mathrm{d}\mathscr{P}}{dy_2} = \exp(-y_2) \tag{20}$$

The histograms are the number of counts in dy. Multiplying by 1000 (the number of counts) and the bin width

$$\Delta y_1 = 0.5 \qquad \Delta y_1 = 0.2 \tag{21}$$

we have

$$\Delta N(y_1) = \frac{500}{y_1^2} \qquad \Delta N(y_2) = 200\exp(-y_2) \tag{22}$$

(c) Based the previous parts we want

$$\frac{dx}{dy} = 3y^2 \tag{23}$$

So that

$$\mathrm{d}\mathscr{P} = 3y^2\,\mathrm{d}y \tag{24}$$

Multipying both sides of Eq. (6) by dy and integrating

$$x = \int_0^y 3y'^2 dy' = y^3 \tag{25}$$

So

$$y = x^{1/3} \tag{26}$$

Indeed looking at the first number in the table $0.536581^{1/3} = 0.812603$.

Problem 5. A reminder on Jacobians

Recall that if I have a probability distribution

$$\mathrm{d}\mathscr{P}_x = P(x)\mathrm{d}x\,, \tag{27}$$

and I want to change variables to a new variable $u(x)$, then the probability distribution for u is

$$\mathrm{d}\mathscr{P}_u = P(x(u))\left|\frac{dx}{du}\right|\mathrm{d}u\,. \tag{28}$$

So the probability densities are arelated by

$$P(u) = P(x(u))\left|\frac{dx}{du}\right|\,. \tag{29}$$

We will have many physical examples of this in homework, e.g. the probability of a particle having a given velocity vs. the probability of a particle having a given energy.

The change of variables generalizes to two and higher dimensions. Suppose we have a probability density in x, y describing a particle's position:

$$\mathrm{d}\mathscr{P}_{x,y} = P(x,y)\,\mathrm{d}x\,\mathrm{d}y\,. \tag{30}$$

For definiteness consider the gaussian

$$\mathrm{d}\mathscr{P}_{x,y} = \frac{1}{2\pi\sigma^2}\exp\left(-\tfrac{x^2}{2\sigma^2} - \tfrac{y^2}{2\sigma^2}\right)\mathrm{d}x\mathrm{d}y\,, \tag{31}$$

shown in Fig. 2. It seems more natural here to use polar coordinates, defining $x = r\cos\theta$ and $y = r\sin\theta$ with $r \in [0,\infty]$ and $\theta \in [0, 2\pi]$ shown in the figure.

In analogy with the 1D case, for a change of variables $x(r,\theta)$ and $y(r,\theta)$, the probability of finding a particle with radius between r and $r + \mathrm{d}r$ and angle θ between θ and $\theta + \mathrm{d}\theta$ is

$$\mathrm{d}\mathscr{P}_{r,\theta} = P(x(r,\theta), y(r,\theta))\left|\left|\frac{\partial(x,y)}{\partial(r,\theta)}\right|\right|\mathrm{d}r\mathrm{d}\theta\,. \tag{32}$$

The double bars mean determinant and then absolute value of the Jacobian matrix, which is defined as a matrix with all the possible derivatives of the map $(r,\theta) \to (x,y)$:[6]

$$\frac{\partial(x,y)}{\partial(r,\theta)} \equiv \begin{pmatrix} \frac{\partial x}{\partial r} & \frac{\partial x}{\partial \theta} \\ \frac{\partial y}{\partial r} & \frac{\partial y}{\partial \theta} \end{pmatrix}\,. \tag{33}$$

So the densities are related by

$$P(r,\theta) = P(x,y)\left|\left|\frac{\partial(x,y)}{\partial(r,\theta)}\right|\right|\,, \tag{34}$$

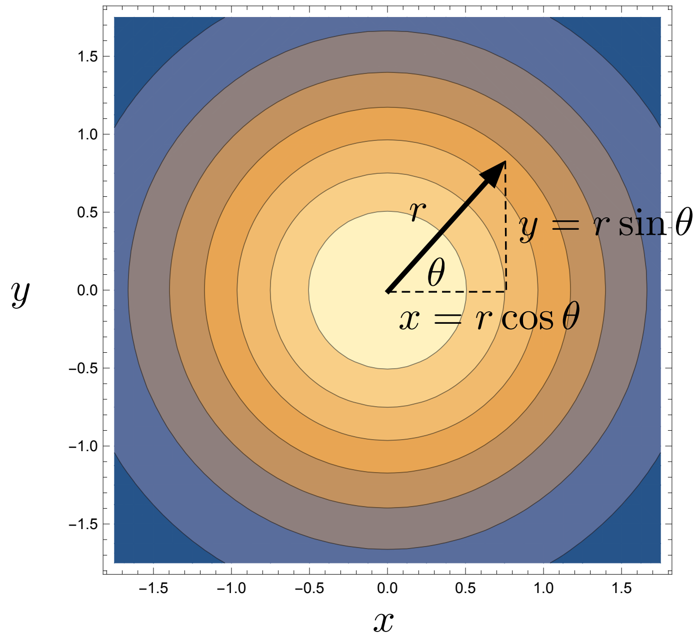


Figure 2: A probability distribution which has no dependence on θ.

where it is understood that $x = r\cos\theta$ and $y = r\sin\theta$.

We say that the "volume elments" are related by the Jacobian determinant:

$$\mathrm{d}x\,\mathrm{d}y = \left|\left|\frac{\partial(x,y)}{\partial(r,\theta)}\right|\right| drd\theta = \ r\,\mathrm{d}r\,\mathrm{d}\theta\,, \tag{35}$$

where it is understood that these expressions are meant to be integrated over.

(a) Compute the Jacobian matrix and find its determinant. Explicitly determine $\mathrm{d}\mathscr{P}_{r,\theta} = P(r,\theta)\mathrm{d}r\mathrm{d}\theta$ for the probability distribution in Eq. (31). By marginalizing over (aka integrating over) the unobserved coordinate, determine $\mathrm{d}\mathscr{P}_r = P(r)\mathrm{d}r$ and $\mathrm{d}\mathscr{P}_\theta = P(\theta)\mathrm{d}\theta$, that is to say the probability distribution for r (without regards to θ) and the probability distribution for θ (without regards to r) ?

(b) Let's understand the Jacobian. The columns of the Jacobian form vectors

$$\boldsymbol{e}_r \equiv \frac{\partial x}{\partial r}\,\hat{\boldsymbol{\imath}} + \frac{\partial y}{\partial r}\,\hat{\boldsymbol{\jmath}} = \frac{\partial \boldsymbol{R}}{\partial r}\,, \tag{36}$$

$$\boldsymbol{e}_\theta \equiv \frac{\partial x}{\partial \theta}\,\hat{\boldsymbol{\imath}} + \frac{\partial y}{\partial \theta}\,\hat{\boldsymbol{\jmath}} = \frac{\partial \boldsymbol{R}}{\partial \theta}\,, \tag{37}$$

where $\boldsymbol{R} = x\hat{\boldsymbol{\imath}} + y\hat{\boldsymbol{\jmath}}$ is the position vector of the particle. The determinant of two vectors is the area of the parallelogram spanned by the two vectors[7]. Compute the

[6] Sometimes people use $\partial(x,y)/\partial(v,\theta)$ to mean the determinant of the Jacobian matrix, rather than just the matrix itself. Our book uses this notation, as is described in appendix C.

[7] See for instance The Kahn video.

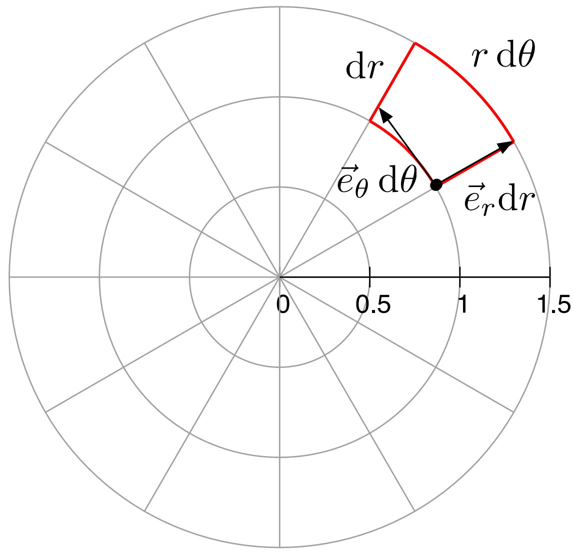


Figure 3: Cylindrical coordinates in two dimensions.

vectors[8] $\boldsymbol{e}_r\,\mathrm{d}r$ and $\boldsymbol{e}_\theta\,\mathrm{d}\theta$, and the norms of the these vectors $|\boldsymbol{e}_r\mathrm{d}r|$ and $|\boldsymbol{e}_\theta\mathrm{d}\theta|$ and show that the vectors are orthogonal in this case. In a sentence or two, use the word "displacement" to explain the physical meaning of the vectors $\boldsymbol{e}_r\mathrm{d}r$ and $\boldsymbol{e}_\theta\mathrm{d}\theta$ and their lengths by referring to Fig. 3. Note that the volume element is $|\boldsymbol{e}_r dr||\boldsymbol{e}_\theta d\theta|$ since the vectors are orthogonal.

Consider the probability distribution

$$\mathrm{d}\mathscr{P}_{x,y} = \frac{1}{6\pi} e^{\left(-5x^2+2xy-2y^2\right)/18}\mathrm{d}x\,\mathrm{d}y \tag{38}$$

A contour plot of this probability distribution is shown in Fig. 4(a). Consider the change of variables

$$x = (u+v) \tag{39}$$
$$y = (-u+2v) \tag{40}$$

The u, v coordinates are better adapted to the probability distribution and are shown in Fig. 4(a).

(c) Compute the Jacobian of the map and compute the probability distribution

$$\mathrm{d}\mathscr{P}_{u,v} = P(u,v)\mathrm{d}u\,\mathrm{d}v \tag{41}$$

Your result should be qualitatively consistent with the contour plot of the result shown in Fig. 4(b).

[8] I am asking for the vector $\boldsymbol{e}_r$ times an (arbitrary) small increment in radial coordinate dr. Weighting $\boldsymbol{e}_r$ and $\boldsymbol{e}_\theta$ by the corresponding coordinate increments dr and $d\theta$ gives these vectors a simple geometric meaning in terms of displacements, which I hope you will begin to understand.

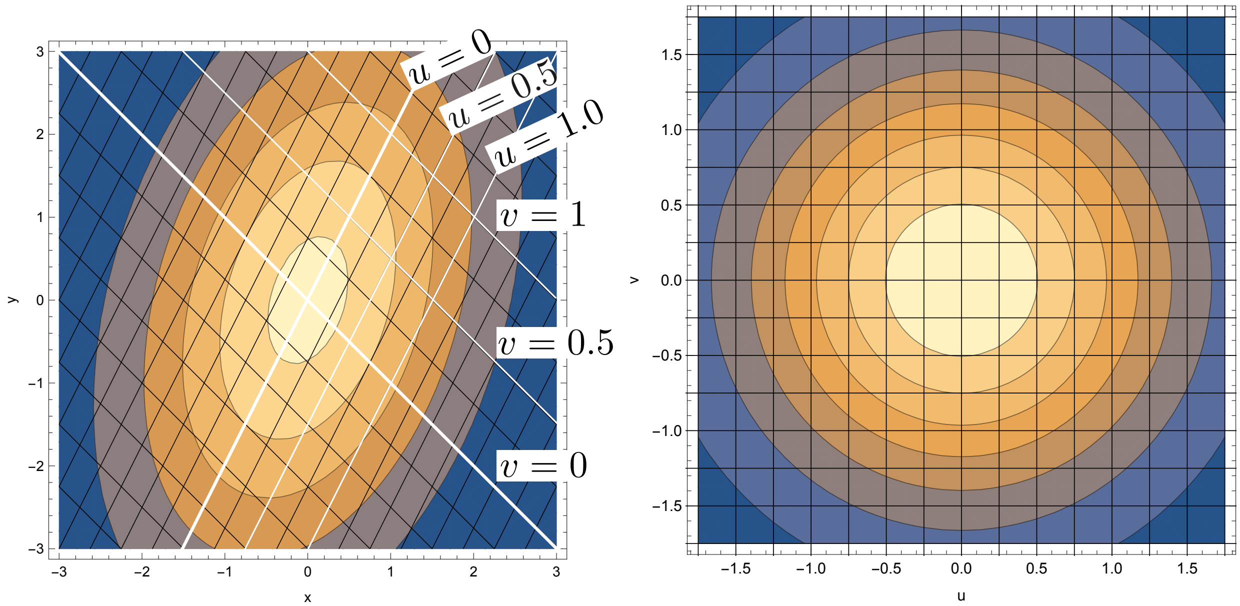


Figure 4: (a) A contour plot of the probability distribution $P(x, y)$ with lines of constant u and v indicated. Specific lines of constant u and v are indicated by the white lines. (b) a contour plot $P(u, v)$ with corresponding lines of constant u and v. The distribution becomes circular for this change of variables.

Show that the probability of finding u in an interval between u and $u + \mathrm{d}u$ is

$$\mathrm{d}\mathscr{P}_u = P(u)\mathrm{d}u \quad \text{with} \quad P(u) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}u^2} . \tag{42}$$

(d) Write down the column vectors, $\boldsymbol{e}_u$ and $\boldsymbol{e}_v$, of the Jacobian of the map $(u, v) \mapsto (x, y)$.

Now interpret these vectors: At the origin of Fig. 4(b), sketch the unit coordinate displacement vectors giving $\Delta u = 1$ and $\Delta v = 1$. At the origin of Fig. 4(a), sketch the corresponding the dispacement vectors $\boldsymbol{e}_u \Delta u$ and $\boldsymbol{e}_v \Delta v$.

Jacobians

a) $x = r\cos\theta \qquad y = r\sin\theta$

$$\begin{bmatrix} \partial x/\partial r & \partial x/\partial \theta \\ \partial y/\partial r & \partial y/\partial \theta \end{bmatrix} = \begin{pmatrix} \cos\theta & -r\sin\theta \\ \sin\theta & r\cos\theta \end{pmatrix}$$

So the determinant is

$$J = \cos^2\theta \cdot r + (\sin^2\theta)\, r = r$$

So

$$\boxed{d\mathcal{P}(r,\theta) = \frac{1}{2\pi\sigma^2} e^{-r^2/2\sigma^2}\, r\, dr\, d\theta}$$

Integrating over θ:

$$d\mathcal{P}(r) = \int_{\text{over-}\theta} d\mathcal{P}(r,\theta) = \frac{1}{2\pi\sigma^2} e^{-r^2/2\sigma^2}\, r\, dr \cdot 2\pi$$

$$\boxed{d\mathcal{P}_r = \frac{1}{\sigma^2} e^{-r^2/2\sigma^2}\, r\, dr}$$

Similarly integrating over r

$$\boxed{d\mathcal{P}_\theta = \int_{\text{over-}r} d\mathcal{P}_{r,\theta} = d\theta \int_0^\infty \frac{1}{2\pi\sigma^2} e^{-r^2/2\sigma^2}\, r\, dr = \frac{d\theta}{2\pi}}$$

b) So

$$\vec{e}_r = \underbrace{\frac{\partial \vec{R}}{\partial r}}_{} = \cos\theta\,\hat{\imath} + \sin\theta\,\hat{\jmath}$$

this vector points in the direction of increasing r

$\vec{e}_r\,dr$ is the change in position $\vec{R}$ with a small change in radius

$$\vec{e}_\theta = \frac{\partial \vec{R}}{\partial \theta} = -r\sin\theta\,\hat{\imath} + r\cos\theta\,\hat{\jmath}$$

So $\vec{e}_\theta\,d\theta$ is the change in position $\vec{R}$ with an increase in angle θ

Note:

- $|\vec{e}_r\,dr| = (\cos^2\theta + \sin^2\theta)^{1/2}\,dr = dr$ ← this is the length of $|\vec{e}_r dr|$
- $|e_\theta\,d\theta| = (r^2\sin^2\theta + r^2\cos^2\theta)^{1/2}\,d\theta = r\,d\theta$

- Then they are orthogonal

$$\vec{e}_r \cdot \vec{e}_\theta = -r\cos\theta\sin\theta + r\cos\theta\sin\theta = 0$$

- Clearly since $\vec{e}_\theta\,d\theta$ is the displacement due to a change of by $d\theta$, the magnitude of this displacement is by geometry $r\,d\theta$, which is confirmed by the math $|\vec{e}_\theta\,d\theta| = r\,d\theta$

- Since the vectors are orthogonal the volume element is

$$dV = |\vec{e}_r\,dr|\,|\vec{e}_\theta\,d\theta| = dr\,(r\,d\theta) = r\,dr\,d\theta$$

c) We have

$$J = \begin{vmatrix} \partial x/\partial u & \partial x/\partial v \\ \partial y/\partial u & \partial y/\partial v \end{vmatrix} = \begin{vmatrix} 1 & 1 \\ -1 & 2 \end{vmatrix} = 3$$

So the arguement of the exponent is

$$-5x^2 + 2xy - 2y^2 = -5(u+v)^2 + 2(u+v)(-u+2v) + 2(-u+2v)(-u+2v)$$

$$= -9u^2 - 9v^2$$

So

$$d\mathcal{P}_{u,v} = \frac{1}{6\pi} \exp\left((-9u^2 - 9v^2)/18\right) \cdot 3\, du\, dv = \frac{1}{2\pi} \exp\left(\frac{-u^2}{2} - \frac{v^2}{2}\right) du\, dv$$

If we don't care about v we integrate over it (aka we "marginalize" over v), so

$$d\mathcal{P}_u = \int_{\text{over-}v} d\mathcal{P}_{u,v} = \frac{e^{-u^2/2}}{2\pi} du \cdot \int_{-\infty}^{\infty} e^{-v^2/2}\, dv$$

$$= \frac{e^{-u^2/2}}{2\pi} du\, \sqrt{2\pi} = \frac{e^{-u^2/2}}{\sqrt{2\pi}}$$

The vectors are

$$\vec{e}_u = \frac{\partial \vec{R}}{\partial u} = \hat{\imath} - \hat{\jmath}$$

$$\vec{e}_v = \frac{\partial \vec{R}}{\partial v} = \hat{\imath} + 2\hat{\jmath}$$

$\vec{e}_u\, du$ is the displacement for given du, at given u, v

$\vec{e}_v\, dv$ is the displacement for given dv, at given u, v

Then at the origin and $du = 1$ $dv = 1$