Problem 1. 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. 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) In class we said that 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:

$$C_p = C_V + \frac{VT\beta_p^2}{\kappa_T}\,. \tag{1}$$

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

$$C_p = C_V + Nk_B\,. \tag{2}$$

Or, for one mole of substance

$$C_p^{1\mathrm{ml}} = C_V^{1\mathrm{ml}} + R\,. \tag{3}$$

Show that Eq. (3) follows from Eq. (1) together with the results from parts (a).

(d) (Optional, but so good) The *adiabatic* compressibility κ_S is the defined by[1]

$$\kappa_S \equiv \frac{-1}{V}\left(\frac{\partial V}{\partial p}\right)_{adiab} \tag{5}$$

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

$$\kappa_S = \frac{\kappa_T}{\gamma} \tag{6}$$

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

Hint: You will need to recall that in an adiabatic change of pressure and volume, we have $pV^\gamma = \text{const}$ for an ideal gas.

[1] 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.

$$\kappa_S \equiv \frac{-1}{V}\left(\frac{\partial V}{\partial p}\right)_S \equiv \frac{-1}{V}\left(\frac{\partial V}{\partial p}\right)_{adiab} \tag{4}$$

(e) As discussed in class, the speed of sound is related to the compressibility[2]

$$c_s = \sqrt{\frac{B_S}{\rho}} \tag{7}$$

where the bulk modulus

$$B_S \equiv -V \left(\frac{\partial p}{\partial_V}\right)_{adiab} \equiv \frac{1}{\kappa_S} \tag{8}$$

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) (Optional, but so good) 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? Why are the best frying pans made of cast iron? Is iron a better heat conductor than air?

[2] 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)

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

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

$$C_p = C_V + Nk \qquad \text{All ideal gasses}$$

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

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

So

$$\gamma = C_p / C_v = 5/2 \, / \, 3/2 = \frac{5}{3} \quad \text{MAI G}$$

$$\gamma = C_p / C_v = 7/2 \, / \, 5/2 = \frac{7}{5} \quad \text{DAI 6}$$

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

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

So

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

$$C_p = C_v + Nk$$

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

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

$$= \left(\frac{\gamma p}{\rho}\right)^{1/2} = \left(\frac{\gamma N k T}{V \rho}\right)^{1/2}$$

$V\rho = mN$

$$c_s = \left(\frac{\gamma k T}{m}\right)^{1/2}$$

$\gamma = \frac{7}{5}$ ← Diatomic!

$m = 28\ m_p$ ← N_2 has 28 nucleons

So

A nucleon is either a proton or a neutron.

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

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

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

For comparison in O_2 gas we have

$C_s \simeq 327\ m/s$

Problem 2. 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, $N_A \cdot \mathrm{eV} = 96.5\,\mathrm{eV}$. 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

$$dH = đQ_{\mathrm{in}} + V\,dp \tag{9}$$

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

$$dH = đQ_{\mathrm{in}} \tag{10}$$

(b) Consider the combustion of Hydrogen gas:

$$\mathrm{H_2}(g) + \frac{1}{2}\mathrm{O_2}(g) \leftrightarrow \mathrm{H_2O}(l)\,. \tag{11}$$

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[3] in the accompanying data table. Determine the change in enthalpy, $\Delta H^{\ominus}$, 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, $\Delta U^{\ominus} = U_{\mathrm{final}} - U_{\mathrm{initial}}$, per mole. (Ans: $Q_{\mathrm{out}} = 285.8\,\mathrm{kJ}$ and $\Delta U = -282.1\,\mathrm{kJ}$)

(c) Consider the reaction at

$$\mathrm{H}(g) + \mathrm{H}(g) \rightarrow \mathrm{H_2}(g) \tag{12}$$

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:

$$E_{\mathrm{H_2}} = \mathrm{KE} + \mathrm{PE} = \mathrm{KE} - \Delta \tag{13}$$

[3] This temperature and pressure is the so-called Normal Temperature and Pressure (NTP) and denoted with a circle, i.e. $T^{\ominus}$, $p^{\ominus}$ and $H^{\ominus}$ denote the temperature, pressure, and enthalpy at NTP.

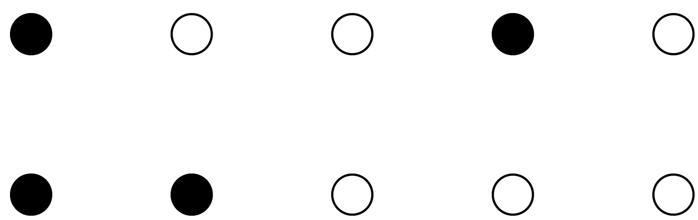
Here PE $= -\Delta$ is the binding energy (i.e. the bond energy) of the two atoms. (The negative sign indicates that the energy is lower when the two atoms are bound compared to when they are unbound. Δ is a positive value and is what we are trying to find.) The total energy U is the sum of kinetic and 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.

Problem 3. 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

$$\Omega = 10^{1.67\times 10^{23}} \tag{14}$$

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

$$\ln\Omega = -\sum_{i=1,2} N_i \ln(N_i/N) \tag{15}$$

$$= N\sum_{i=1,2} -P_i \ln P_i \tag{16}$$

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[4]. Then entropy per site, i.e. $\ln\Omega/N$, is given by

$$\frac{\ln\Omega}{N} = \sum_i -P_i \ln P_i \tag{17}$$

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.

[4] 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 4. Central Limit Theorem and Random Walk

In a random walk, a collegiate drunkard starts at the origin and takes a step of size a, to the right with probability p and to the left with probability $1-p$.

(a) Take $p = 1/2$, i.e. equal probability of right and left steps. Determine the probability of the drunkard having position X, i.e. $P(X)$, after three steps. Plot $P(X)$ where X can be one of $X = 0, \pm 1, \pm 2, \pm 3$. Note how your graph begins to approach a Gaussian after just three steps.

(b) Now keep p general. What is the mean and variance variance in the drunkard's position X after one step, and after two steps?

(c) After n steps (with $n \gg 1$) find his mean position $\langle X \rangle$, and the std. deviation in his position $\sigma_X = \sqrt{\langle \delta X^2 \rangle}$. Check your result by comparing with the figure below

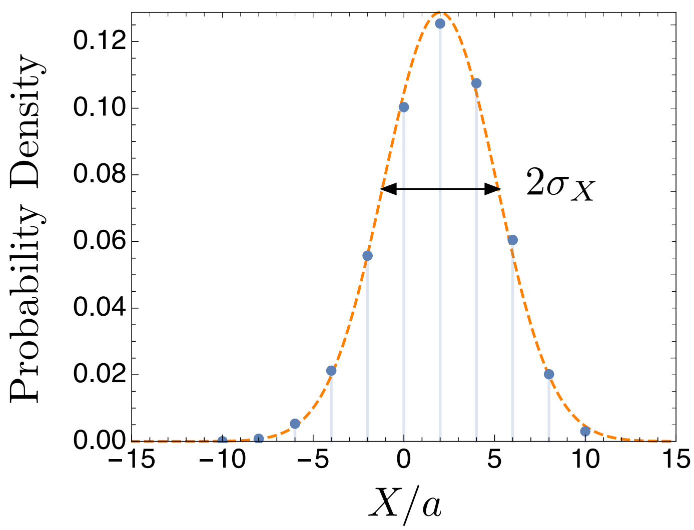


Figure 1: Probability of our drunkard having position X after $n = 10$ steps (the blue points). Of course after 10 steps the drunkard will be between $-10 \ldots 10$, and it is easy to show that he will be only at the even sites, i.e. $-10, -8, -6, \ldots 10$. For $p = 0.6$, I find $\langle X \rangle = 2.0$. Twice the std deviation, $2\sigma_X$, is shown in the figure and is about six in this case. The orange curve is a gaussian (a.k.a the "bell-shaped" curve) approximation discussed in class and approximately agrees with the points – this is the central limit theorem. Recall that the central limit theorm says that if the number of steps n is large, the probability of X (a sum of n independent events) is approximately $P(x)\,dX \propto \exp(-(X - \langle X \rangle)^2/2\sigma_X^2)$. Evidently the gaussian approximation works well already for $n = 10$.

Hint: X is a sum N independent events x_i where $x_i = \pm a$. Use results from class on the probability distribution of a *sum* of independent events.

(d) (Optional. Don't turn in) If p is very nearly $\frac{1}{2}$, say $p = 0.5001$, determine how many steps it will take before the mean value $\langle X \rangle$ is definitely different from zero. By "definitely" I mean that $\langle X \rangle$ is "more than two sigma" away from zero, $\langle X \rangle > 2\sigma_X$. If $p = \frac{1}{2} + \epsilon$ (with ϵ tiny), you should find (approximately) that

$$N_{\text{steps}} \simeq \frac{1}{\epsilon^2} \tag{18}$$

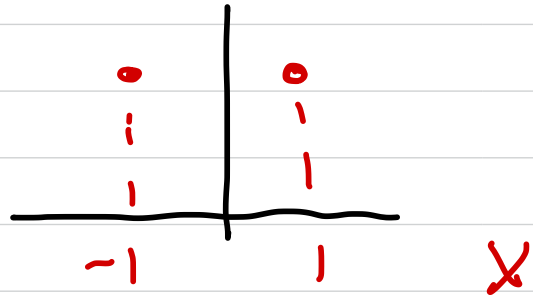
up to corrections of order ϵ. Here $p = \frac{1}{2} + \epsilon$ with $\epsilon = 0.0001$, how does the result scale with ϵ, e.g. if I where two half ϵ how would the number of required steps change?

Random Walk

After 1 step:

$P_1 = 1/2$

$P_{-1} = 1/2$

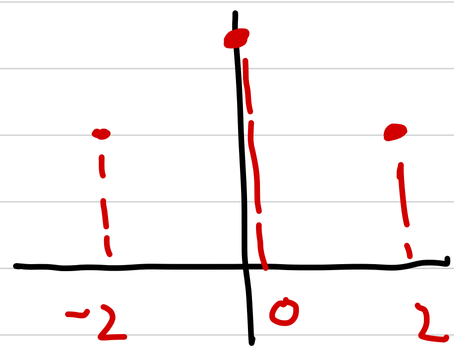


After 2 steps

$$P_2 = \frac{1}{2} \cdot \frac{1}{2} = \frac{1}{4}$$

$$P_0 = \frac{1}{2} \cdot \frac{1}{2} + \frac{1}{2} \cdot \frac{1}{2} = \frac{1}{2}$$

$$P_{-2} = \frac{1}{2} \cdot \frac{1}{2} = \frac{1}{4}$$



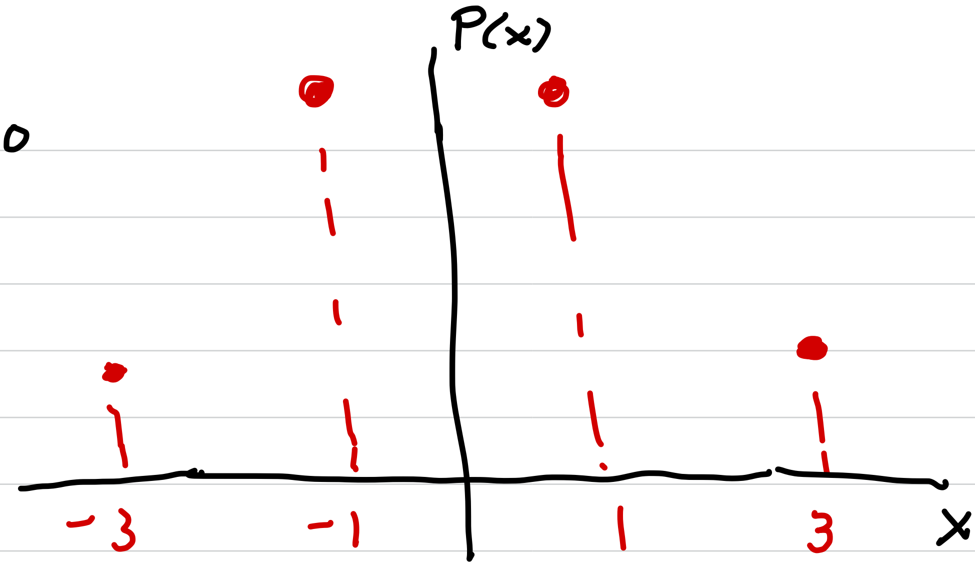
After 3 steps

$$P_3 = \frac{1}{4} \cdot \frac{1}{2} = \frac{1}{8}$$

$$P_1 = \frac{1}{4} \cdot \frac{1}{2} + \frac{1}{2} \cdot \frac{1}{2} = \frac{3}{8}$$

$$P_{-1} = \frac{3}{8}$$

$P_{-3} = \frac{1}{8}$, So



b) The mean and variance for one step are:

$$\overline{x} = a p - (1-p) a = a(2p-1) = \overline{x}_1$$

$$\overline{x^2} = a^2 p + (1-p) a^2 = a^2 = \delta x^2$$

$$\langle \delta x^2 \rangle = \overline{x}^2 - \overline{x}^2 = a^2 - a^2 (2p-1)^2$$

$$= a^2 (1 - ((2p)^2 - 2(2p) + 1)) = 4a^2 p(1-p)$$

Now the mean and variance add

$$\left.\begin{aligned} \overline{X}_2 &= 2\overline{x} = 2a(2p-1) \\ \langle \delta X_2^2 \rangle &= 2\langle \delta x^2 \rangle = 8a^2 p(1-p) \end{aligned}\right\} \text{two steps are twice one step}$$

c) Now for part (c)

$$\bar{X}_N = N a (2p-1)$$

For $N=10$ $p=0.6$ $\bar{X}_N = 10\,(2\;0.6-1) = 2$

This clearly agrees with the figure wich is centered at $X/a = 2$

Similarly we compute the variance

$$\langle \delta X_N^2 \rangle = 4N\,a^2\,p(1-p) \quad \text{for } N=10 \quad p=0.6$$

we find $\langle \delta X_N^2 \rangle \simeq 9.6$ so $\sigma \equiv \sqrt{\langle \delta X^2 \rangle} \simeq 3.1$

Comparison with the graph gives $2\sigma \simeq 6.2$ which seems about right.

d) The mean is $Na(1-2p) = \langle X \rangle$. The standard deviation is $\sigma_x = \sqrt{N}\,2a\,(p(1-p))^{1/2}$. Requiring that $\langle X \rangle > 2\sigma_x$ gives

$$N\,(1-2p) > 2\sqrt{N}\,(4\,p(1-p))^{1/2}$$

Solving for N we have

$$N > \frac{16\,p(1-p)}{(1-2p)^2}$$

So for $p = 1/2 + \varepsilon$, we have

$$N > \frac{16\,\frac{1}{2}(1-\frac{1}{2})}{(2\varepsilon)} \simeq \frac{1}{\varepsilon^2}$$

Problem 5. A reminder on Jacobians

Recall that if I have a probability distribution

$$\mathrm{d}\mathscr{P}_x = P(x)\mathrm{d}x\,, \tag{19}$$

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

$$\mathrm{d}\mathscr{P}_u = P(x(u))\left|\frac{dx}{du}\right|\mathrm{d}u\,. \tag{20}$$

So the probability densities are arelated by

$$P(u) = P(x(u))\left|\frac{dx}{du}\right|\,. \tag{21}$$

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:

$$\mathrm{d}\mathscr{P}_{x,y} = P(x,y)\,\mathrm{d}x\,\mathrm{d}y\,. \tag{22}$$

For definiteness consider the gaussian

$$\mathrm{d}\mathscr{P}_{x,y} = \frac{1}{2\pi\sigma^2}\exp\left(-\tfrac{x^2}{2\sigma^2} - \tfrac{y^2}{2\sigma^2}\right)\mathrm{d}x\mathrm{d}y\,, \tag{23}$$

shown in Fig. **??**. 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

$$\mathrm{d}\mathscr{P}_{r,\theta} = P(x(r,\theta), y(r,\theta))\left\|\frac{\partial(x,y)}{\partial(r,\theta)}\right\|\mathrm{d}r\mathrm{d}\theta\,. \tag{24}$$

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 $(r,\theta) \to (x,y)$:[5]

$$\frac{\partial(x,y)}{\partial(r,\theta)} \equiv \begin{pmatrix} \frac{\partial x}{\partial r} & \frac{\partial x}{\partial \theta} \\ \frac{\partial y}{\partial r} & \frac{\partial y}{\partial \theta} \end{pmatrix}\,. \tag{25}$$

So the densities are related by

$$P(r,\theta) = P(x,y)\left\|\frac{\partial(x,y)}{\partial(r,\theta)}\right\|\,, \tag{26}$$

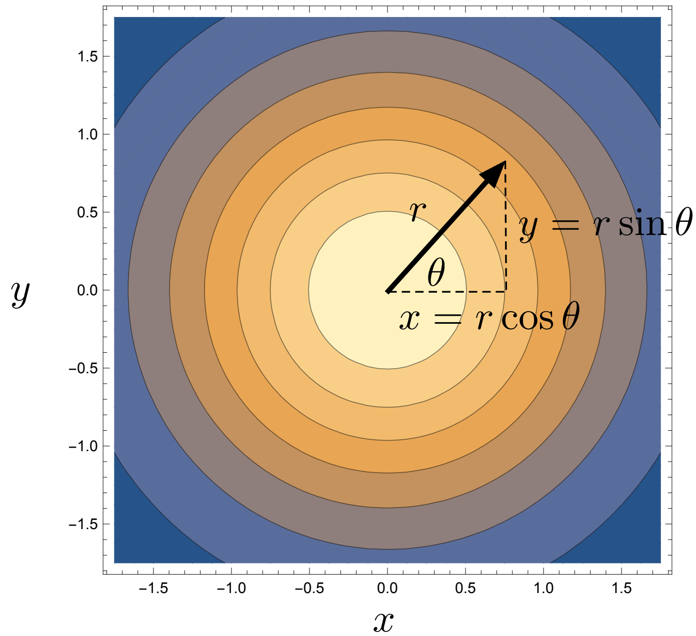


Figure 2: A probability distribution which has no dependence on θ.

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:

$$\mathrm{d}x\,\mathrm{d}y = \left|\left|\frac{\partial(x,y)}{\partial(r,\theta)}\right|\right| drd\theta = \; r\,\mathrm{d}r\,\mathrm{d}\theta\,, \tag{27}$$

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. (**??**). 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

$$\boldsymbol{e}_r \equiv \frac{\partial x}{\partial r}\,\hat{\boldsymbol{\imath}} + \frac{\partial y}{\partial r}\,\hat{\boldsymbol{\jmath}} = \frac{\partial \boldsymbol{R}}{\partial r}\,, \tag{28}$$

$$\boldsymbol{e}_\theta \equiv \frac{\partial x}{\partial \theta}\,\hat{\boldsymbol{\imath}} + \frac{\partial y}{\partial \theta}\,\hat{\boldsymbol{\jmath}} = \frac{\partial \boldsymbol{R}}{\partial \theta}\,, \tag{29}$$

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[6]. Compute the

[5]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.

[6]See for instance The Kahn video.

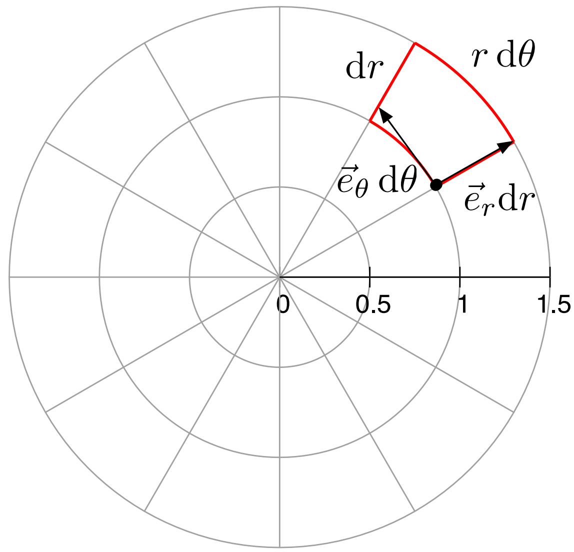


Figure 3: Cylindrical coordinates in two dimensions.

vectors[7] $\boldsymbol{e}_r\,\mathrm{d}r$ 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. **??**. Note that the volume element is $|\boldsymbol{e}_r dr||\boldsymbol{e}_\theta d\theta|$ since the vectors are orthogonal.

Consider the probability distribution

$$\mathrm{d}\mathscr{P}_{x,y} = \frac{1}{6\pi} e^{\left(-5x^2+2xy-2y^2\right)/18}\mathrm{d}x\,\mathrm{d}y \tag{30}$$

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

$$x = (u+v) \tag{31}$$
$$y = (-u+2v) \tag{32}$$

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

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

$$\mathrm{d}\mathscr{P}_{u,v} = P(u,v)\mathrm{d}u\,\mathrm{d}v \tag{33}$$

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

[7] 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.

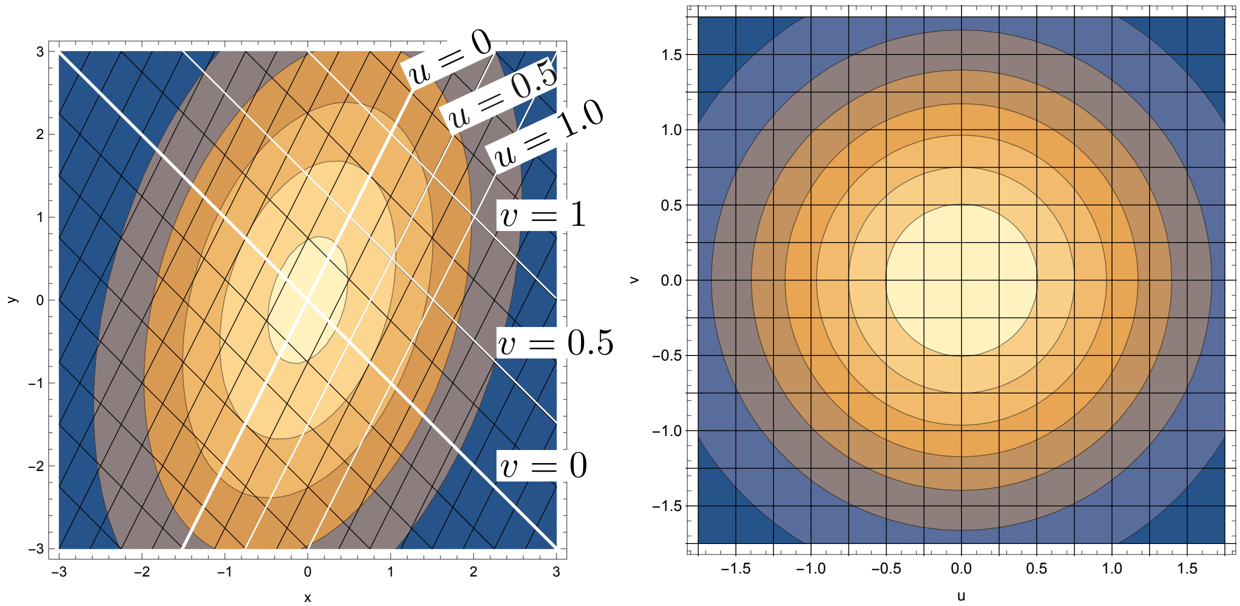


Figure 4: (a) A contour plot of the probability distribution $P(x, y)$ with lines of constant u and v indicated. Specific lines of constant u and v are indicated by the white lines. (b) a contour plot $P(u, v)$ with corresponding lines of constant u and v. The distribution becomes circular for this change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

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

$$\mathrm{d}\mathscr{P}_u = P(u)\mathrm{d}u \quad \text{with} \quad P(u) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}u^2} \,. \tag{34}$$

(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. **??**(b), sketch the unit coordinate displacement vectors giving $\Delta u = 1$ and $\Delta v = 1$. At the origin of Fig. **??**(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

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

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 $du = 1$ $dv = 1$