Problem 1. Distributions on the sphere

- (a) Consider a particle with angular coordinates (θ, ϕ) which are uniformly distributed over a sphere of radius R, i.e. the probability per area is constant. Briefly explain (using the definition of solid angle) why $d\mathscr{P} = Cd\Omega$ with C a normalizing constant. Determine C and show that the probability distribution per $d\theta$ is $d\mathscr{P} = \frac{1}{2}\sin\theta d\theta$. Show that $\langle \cos^2 \theta \rangle_{\text{sphere}} = \frac{1}{3}$.
- (b) Consider a particle which is distributed (not uniformly) over the sphere

$$d\mathscr{P} = C(1 + \cos^2 \theta) \frac{\mathrm{d}\Omega}{4\pi} \tag{1}$$

where C is a normalizing constant. This probability distribution is visualized in Fig. 1. Show that C = 3/4. Then show that the probability distribution in Eq. (1), implies that the probability distribution for $u = \cos(\theta)$ is

$$d\mathscr{P} = \frac{3}{8}(1+u^2)\,\mathrm{d}u\tag{2}$$

for $u \in [-1, 1]$.

(c) Show for the probability distribution of (b) that $\langle \cos^2 \theta \rangle_{\text{sphere}} = \frac{2}{5}$ by averaging $\langle u^2 \rangle$ with the distribution in Eq. (2).

Two takeaway morals:

• Moral 1: $4\pi = 2 \cdot 2\pi$, the spherical measure factorizes into two properly normalized probability distributions for θ and ϕ :

$$\frac{\mathrm{d}\Omega}{4\pi} = \frac{\sin\theta \,\mathrm{d}\theta \,\mathrm{d}\phi}{4\pi} = P(\theta) \,\mathrm{d}\theta \,P(\phi) \,\mathrm{d}\phi = \left(\frac{1}{2}\sin\theta \,\mathrm{d}\theta\right) \left(\frac{\mathrm{d}\phi}{2\pi}\right) \tag{3}$$

So if you don't care about the about the azimuthal direction and only want to know about the probability of θ , one has the measure $d\mathscr{P} = \frac{1}{2}\sin\theta d\theta$.

• Moral 2: When integrating over the sphere it is almost always better to integrate over $u = \cos \theta$, so that the measure is flat $d\Omega = du d\phi$.

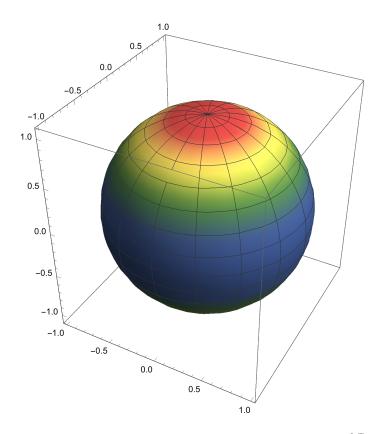


Figure 1: A visualization of a probability distribution on a sphere $\frac{d\mathscr{P}}{d\Omega} \propto (1 + \cos^2 \theta)$. The colors are proportional to the probability per area or per solid angle (since $dA \propto d\Omega$ these are the same).

Problem 2. Density of gas at constant temperature with gravity

In this problem we will do two things:

- We will start to use momentum instead of velocity. This is preferred for reasons that are hard to explain at this level. If you didn't do the optional problem from last week, at least look at part (a). Takes just a second.
- We will give an example where the energy depends on coordinates (x, y, z) and momenta.

Consider a gas at temperature T near the earths surface. The energy (or Hamiltonian) of a molecule with momentum $\mathbf{p} = (p_x, p_y, p_z)$ and coordinate $\mathbf{r} = (x, y, z)$ is

$$E = mgz + \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m} \tag{4}$$

where z=0 is the surface of the earth. The probability of finding a gas molecule with coordinate between $\mathbf{r}=(x,y,z)$ and $\mathbf{r}+\mathrm{d}\mathbf{r}$ (with $\mathrm{d}\mathbf{r}=(dx,dy,dz)$) and momentum between \mathbf{p} and $\mathbf{p}+\mathrm{d}\mathbf{p}$

$$d\mathscr{P} = Ce^{-E/k_BT} d^3 \boldsymbol{r} d^3 \boldsymbol{p} \tag{5}$$

where

$$d^{3}\mathbf{r}d^{3}\mathbf{p} = (dxdydz)(dp_{x}dp_{y}dp_{z})$$
(6)

The quantity is $d^3 \mathbf{r} d^3 \mathbf{p}$ is known as the *phase space* volume element. It records the volume in the "space" of positions and momenta – and this position and momentum "space" is called *phase space*.

(a) For simplicity consider the coordinates x, y, z to be constrained to an (essentially infinitely) large volume $V = L^3$, i.e. $\int d^3 \mathbf{r} = L^3$. Without gravity we found that the probability distribution for position and momenta is

$$d\mathscr{P} = \frac{1}{V} \left(\frac{1}{2\pi m k_B T} \right)^{3/2} e^{-p^2/2m k_B T} d^3 \boldsymbol{r} d^3 \boldsymbol{p}$$
 (7)

The d^3r/V says that the particle is equally likely to be anywhere in the box. If gravity is included, what is the normalization constant C in Eq. (5) and what is $P(z) \equiv \frac{d\mathscr{P}}{dz}$? Consider z ranging from $(0, \infty)$, instead of (0, L).

You can check your result by checking that the dimensions are correct.

(b) Show that the mean height of a molecule of air is $\langle h \rangle = k_B T/mg$. (Intuitively the mean height can be estimated, by estimating when the potential energy mgh becomes comparable to the thermal energy $k_B T$.) Make a reasonable estimate for this height in kilometers, by estimating the typical mass of an air molecule, and a typical temperature.

¹The Hamiltonian is the energy of the system expressed as a functions of r and p

Please do not substitute, $k_B = 1.38 \times 10^{-23} \text{J/°K}^{-1}$, and try not to look up numbers. Rather puts the numbers in physical terms, and remember them. For instance using $R = N_A k_B = 8.32 \, \text{J/°K}$. A list of useful constants that you need for this course is maintained on the web site.

- (c) If the gas density at z = 0 is n_0 , what is the density n(z) at height z?
- (d) A mechanical analysis of the forces in the the gas says that

$$\frac{dp(z)}{dz} = -mgn(z) \tag{8}$$

where p(z) is the pressure in the gas at height z. Explain briefly the physical meaning of Eq. (8), and then show that part (c) is consistent with Eq. (8) and the ideal gas law, $pV = n_{\rm ml}RT$ provided the temperature is constant.

Problem 3. Probability distribution of a Quantum Harmonic Oscillator

Consider a quantum harmonic oscillator in one dimension interacting with a thermal environment. This could be, for example, a single atom attached via a spring-like bond to a large stationary molecule. The vibrational frequency of the oscillator is $\omega_0 = \sqrt{k/m}$.

Recall that the energy levels of a quantum harmonic oscillator are

$$\epsilon_n = \left(n + \frac{1}{2}\right)\hbar\omega_0\tag{9}$$

with $n = 0, 1, 2, \ldots \hbar \omega_0$ is one quantized unit of vibrational energy. The integer n is known as the vibrational quantum number – the larger is n, the larger is the energy (in units of $\hbar \omega_0$), and the more the atom is vibrating. For large n the energy is nearly continuous and the motion can be treated classically. A plot of the energy levels and the wave-functions are shown in Fig. 2.

Since only differences in energies are physically important, we can shift what we call "zero energy" downward by $\frac{1}{2}\hbar\omega_0$ and write the energy levels as

$$\epsilon_n = n\hbar\omega_0 \tag{10}$$

The probability to find the oscillator in the n-th vibrational state is

$$P_n = \frac{1}{Z}e^{-\epsilon_n/k_BT} = \frac{1}{Z}e^{-n\hbar\omega_0/k_BT} \tag{11}$$

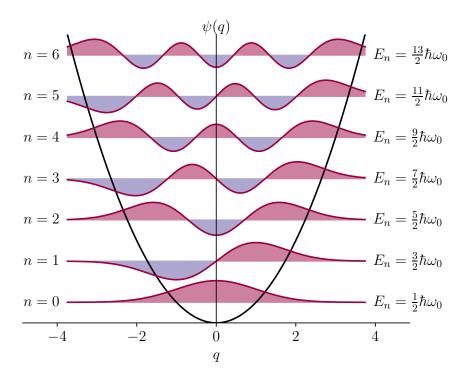


Figure 2: Energy levels $\epsilon_n \equiv E_n = (n + \frac{1}{2})\hbar\omega_0$ and wave functions for the first six levels of the quantum harmonic oscillator.

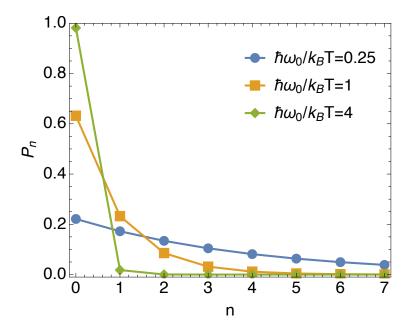


Figure 3: Probability for the oscillator to have n quanta of vibrational energy $\hbar\omega_0$ for different values $\hbar\omega_0/k_BT$.

where Z is a normalizing constant. Z is known as the partition function in English, and the letter Z is short for Zustandsumme in German (meaning sum over states).

- (a) For the probabilities to be correctly normalized, show that $Z = \sum_{n=0}^{\infty} e^{-n\beta\hbar\omega_0}$. I find the German name descriptive, because, as you should see, it is a "sum over states".
- (b) Noting that $e^{-n\hbar\omega_0/k_BT} = u^n$ with $u = e^{-\hbar\omega_0/k_BT}$, evaluate the sum, and determine the explicit form for Z and P_n . A plot of P_n for a variety of $\hbar\omega_0$ is shown in Fig. 3. Describe qualitatively what this plot is telling you physically.

You should find

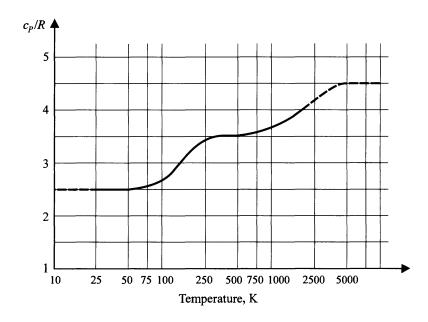
$$P_n = e^{-n\hbar\omega_0/k_BT} (1 - e^{-\hbar\omega_0/k_BT}) \tag{12}$$

(c) The first vibrational excited state (n = 1) of diatomic hydrogen H_2 is excited from the ground state (n = 0) by a photon of wavelength of $\lambda_0 = 2270 \,\mathrm{nm}$. This wavelength is typical of molecular vibrations – is the photon, if rared, visible, or uv? Express the vibrational unit of energy $\hbar\omega_0$ in eV. By looking at Fig. 3, give a rough estimate for the temperature when the mean number of vibrational quanta of energy in the oscillations of H_2 becomes of order unity.

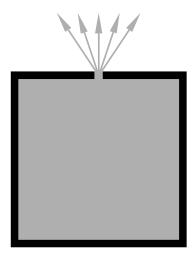
Please do use constants like $\hbar = 1.05 \times 10^{-34} \, \mathrm{J} \, \mathrm{s}$ and $k_B = 1.38 \times 10^{-23} \, \mathrm{J/^\circ K^{-1}}$, but rather try to put it in physical terms. For instance use $\hbar c = 197 \, \mathrm{eV} \, \mathrm{nm}$, and $k_B T \simeq 1/44 \, \mathrm{eV}$ at freezing 273 °K. A summary of constants you will need for the course are given on the website.

Discussion: I find $T \simeq 6000^{\circ}$ K. Indeed this is about right. At room temperatures diatomic molecules translate and rotate so $\langle \epsilon \rangle = \frac{5}{2} k_B T$. At higher temperatures (at

around 1000° K) they begin to vibrate, and the $\frac{5}{2}k_BT$ estimate for the molecule's energy is no longer valid. Much above this temperature the molecule begins to break apart as the number of vibrational quanta gets larger and larger. The following figure shows the specific heat of H_2 gas. As we will discuss fully later, the increase increase starting at around 1000° K reflects the fact vibrational degrees of freedom becoming active, i.e. that the mean n is becoming greater than one.



Problem 4. Probabilities for escaping particles



In class we showed the number of particles per area per second passing through a hole in the container with speeds between (v, v + dv), and angles between $(\theta, \theta + d\theta)$ and $(\phi, \phi + d\phi)$ is

$$d\Phi = nP(v) v \cos\theta \, dv \, \frac{d\Omega}{4\pi} \,. \tag{13}$$

with $d\Omega = \sin \theta d\theta d\phi$.

(a) Show that the total number of particles passing through the hole per are per time is

$$\Phi = \frac{1}{4} n \langle v \rangle \tag{14}$$

For reference $\langle v \rangle = (8k_BT/\pi m)^{1/2}$ but you do not need to show this for this probelm.

- (b) Show that the average value of $\cos \theta$ for these particles is 2/3.
- (c) Your bicycle tire has a slow leak, so that it goes flat within about an $\tau \simeq 1$ hour after being fully inflated. Make an estimate for the radius of the hole when the tire is fully inflated. Take any reasonable estimate for the volume of an inflated tire, the temperature, and a typical mass for air.

Hint: show that the loss of atoms per time takes the form $dN/dt = -N/\tau$, where $\tau^{-1} \equiv A(k_BT/2\pi m)^{1/2}/V$ is a characteristic decay time, and $A = \pi R^2$.

For reasonable estimates of the volume and temperature I find a hole radius of about $R \sim 30$ microns. But of course if your results could differ from mine by factors of two or three.

Problem 5. 2D World

Consider a mono-atomic ideal gas in a two dimensional world, so the velocities are labeled by $\mathbf{v} = (v_x, v_y)$.

(a) Use Jacobians to show that the "volume element" is

$$dv_x dv_y = \left| \left| \frac{\partial(v_x, v_y)}{\partial(v, \theta)} \right| \right| dv d\theta = v dv d\theta$$
 (15)

where $v_x = v \cos \theta$ and $v_y = v \sin \theta$, with $v \in [0, \infty]$ and $\theta \in [0, 2\pi]$. It is understood that these expressions are meant to be integrated over. The double bars mean determinant and then absolute value of the Jacobian matrix, which is defined as²

$$\frac{\partial(v_x, v_y)}{\partial(v, \theta)} \equiv \begin{pmatrix} \frac{\partial v_x}{\partial v} & \frac{\partial v_x}{\partial \theta} \\ \frac{\partial v_y}{\partial v} & \frac{\partial v_y}{\partial \theta} \end{pmatrix}$$
(16)

This generalizes the usual 1d change of variables

$$dx = \left| \frac{dx}{du} \right| du \tag{17}$$

(b) Lets understand the Jacobian. Consider the change of coordinates from $x = r \cos \theta$ and $y = r \sin \theta$. Write down the Jacobian in analogy with (a). The columns of the Jacobian form vectors

$$\boldsymbol{e}_r \equiv \frac{\partial x}{\partial r} \,\hat{\boldsymbol{\imath}} + \frac{\partial y}{\partial r} \,\hat{\boldsymbol{\jmath}} \tag{18}$$

$$\boldsymbol{e}_{\theta} \equiv \frac{\partial x}{\partial \theta} \,\hat{\boldsymbol{\imath}} + \frac{\partial y}{\partial \theta} \,\hat{\boldsymbol{\jmath}}. \tag{19}$$

The determinant of two vectors is the area of the parallelogram spanned by the two vectors³. Compute the norms of these vectors $|\mathbf{e}_r dr|$ and $|\mathbf{e}_\theta d\theta|$ and show that the vectors are orthogonal. Qualitatively interpret these vectors and their lengths by referring to Fig. 4. Note that the volume element is $|\mathbf{e}_r dr| |\mathbf{e}_\theta d\theta|$ since the vectors are orthogonal.

(c) (Optional, but good) In three dimensions, the Jacobian of the map $x = r \sin \theta \cos \phi$, $y = r \sin \theta \sin \phi$, $z = r \cos \theta$, is

$$d^{3}x = \left| \left| \frac{\partial(x, y, z)}{\partial(r, \theta, \phi)} \right| \left| dr d\theta d\phi = \left| \begin{vmatrix} \sin \theta \cos \phi & r \cos \theta \cos \phi & -r \sin \theta \\ \sin \theta \sin \phi & r \cos \theta \sin \phi & r \sin \theta \\ \cos \theta & -r \sin \theta & 0 \end{vmatrix} \right| = r^{2} \sin \theta dr d\theta d\phi$$
(20)

Look at the columns and find the lengths of the collumn vectors, $\mathbf{e}_r dr$, $\mathbf{e}_\theta d\theta$ and $\mathbf{e}_\phi d\phi$. Interpret these vectors and lengths by looking at Fig. 5 where the spherical coordinates explained.

²Sometimes people use $\partial(v_x, v_y)/\partial(v, \theta)$ 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.

³See for instance The Kahn video.

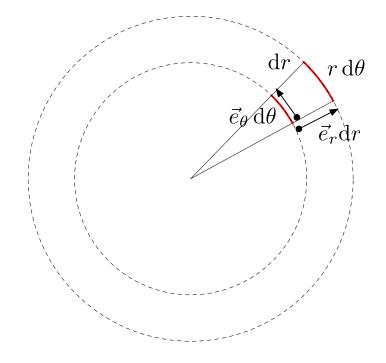


Figure 4: Cylindrical coordinates in two dimensions.

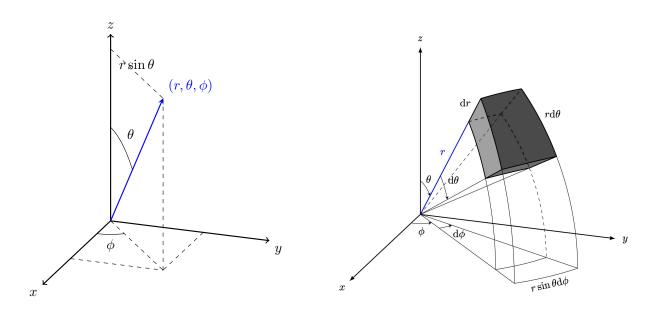


Figure 5: Spherical coordinates.

(d) Write down the normalized Maxwell velocity distribution, $d\mathcal{P}(v_x, v_y) = P(v_x, v_y) dv_x dv_y$, and, using the Jacobian of part (a) and an integral over θ , determine the normalized speed distribution

$$d\mathscr{P}(v) = P(v)dv \tag{21}$$

Describe in plain speak and a simple picture (like Fig. 4) what we are doing with the whole "Jacobian + integral over θ " steps.

You should find that all factors of π have canceled in your final expression for P(v) in two dimensions. You can check your result by doing the next item.

- (e) Compute $\langle \frac{1}{2}mv^2 \rangle$ using the speed distribution. You should find k_BT . Is your result consistent with the equipartition theorem? Explain.
 - Please be explicit about how to do the integral. If you get stuck try changing variables to a dimensionless energy.
- (f) Consider a box of gas with N particles and density n. The box has a small hole. In three dimensions we found that the total flux (number per area per time) escaping the hole is

$$\Phi = \frac{1}{4}n\langle v\rangle \tag{22}$$

and the pressure is determined by $\langle v^2 \rangle$ via

$$p = \frac{1}{3} nm \left\langle v^2 \right\rangle \tag{23}$$

where n is the density. Show that the two dimensional version of these results is

$$\Phi = \frac{1}{\pi} n \langle v \rangle \tag{24}$$

$$p = \frac{1}{2} nm \left\langle v^2 \right\rangle \tag{25}$$

where Φ is the flux (number per length per second). The first step is to find the differential flux $d\Phi$ in two dimensions, generalizing Eq. (13) which is for three dimensions.

Discussion: In two dimensions we have, $\langle v \rangle = (\pi k_B T/2m)^{1/2}$ and $\langle v^2 \rangle = 2k_B T/m$, so the results of part (e) establish that:

$$p = nk_B T \tag{26}$$

$$\Phi = \frac{p}{\sqrt{2\pi m k_{\scriptscriptstyle B} T}} \tag{27}$$

It is noteworthy that these last relations are the same as their 3D counterparts. Indeed, other derivations (see our Book problem 6.9) make it clear that these last relations hold in all dimensions.