Problem 1.   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 4 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 $\boldsymbol{p} = (p_x, p_y, p_z)$ and coordinate $\boldsymbol{r} = (x, y, z)$ is[1]

$$E = mgz + \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m} \tag{1}$$

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

$$d\mathscr{P} = C e^{-E/k_B T} \mathrm{d}^3\boldsymbol{r}\, \mathrm{d}^3\boldsymbol{p} \tag{2}$$

where

$$\mathrm{d}^3\boldsymbol{r}\mathrm{d}^3\boldsymbol{p} = (\mathrm{d}x\mathrm{d}y\mathrm{d}z)\,(\mathrm{d}p_x\mathrm{d}p_y\mathrm{d}p_z) \tag{3}$$

The quantity is $\mathrm{d}^3\boldsymbol{r}\mathrm{d}^3\boldsymbol{p}$ 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. $\int \mathrm{d}^3\boldsymbol{r} = L^3$. Without gravity we found that the probability distribution for position and momenta is

$$d\mathscr{P} = \frac{1}{V}\left(\frac{1}{2\pi m k_B T}\right)^{3/2} e^{-p^2/2mk_B T} \mathrm{d}^3\boldsymbol{r}\, \mathrm{d}^3\boldsymbol{p} \tag{4}$$

The $d^3\boldsymbol{r}/V$ 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. (2) 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 the typical mass of an air molecule, and a typical temperature.

Try to remember the relevant numbers rather than substituting $k_B = 1.38 \times 10^{-23} J/K^{-1}$. For instance use $R = N_A k_B = 8.32 J/°K$ and $N_A m =$ molar-mass. My basic feeling is that if you have to look up a number you don't understand something fundamental.

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[1]The Hamiltonian is the energy of the system expressed as a functions of $\boldsymbol{r}$ and $\boldsymbol{p}$

(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

$$\frac{dp(z)}{dz} = -mgn(z) \tag{5}$$

where $p(z)$ is the pressure in the gas at height z. Explain briefly the physical meaning of Eq. (5), and then show that part (c) is consistent with Eq. (5) and the ideal gas law, $pV = n_{\mathrm{ml}}RT$ provided the temperature is constant.

Problem 2.   Volume of Phase Space: Part I

The purpose is here to get started, talking about the accessible phase space volume. The phase space volume is a measure of the total number of possible ways for a N of particles to share *share* (or partition) the total energy. For instance one particle could have almost all the availble energy and the remaining $N - 1$ could have very little. That possibility occupies only a small portion of the available phase space volume (even for two particles).

(a) Consider a single particle in three dimensions in a box

$$0 < x, y, z < L \tag{6}$$

The three momenta components are *sharing* (or partitioning) the total energy which lies between E and $E + \delta E$, i.e.

$$E < \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m} < E + \delta E, \tag{7}$$

The particle is free to move around in phase space but the energy must lie in this range. Show that the total phase space volume which is available to be shared amongst the three degrees of freedom p_x, p_y, p_z is

$$V_{\mathrm{ps}} = \int_E^{E+\delta E} \mathrm{d}^3 \boldsymbol{r} \, \mathrm{d}^3 \boldsymbol{p} = V(2mE)^{3/2} \, 4\pi \frac{\delta E}{2E} \tag{8}$$

with $V = L^3$.

Hint: The momenta are confied to a spherical shell of radius p_0 in the p_x, p_y, p_z space. How is p_0 related to the energy? If the energy is the between $[E, E + \delta E]$, how is the thickness of the shell δp_0 is related to δE?

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 to a large molecule in a gas.
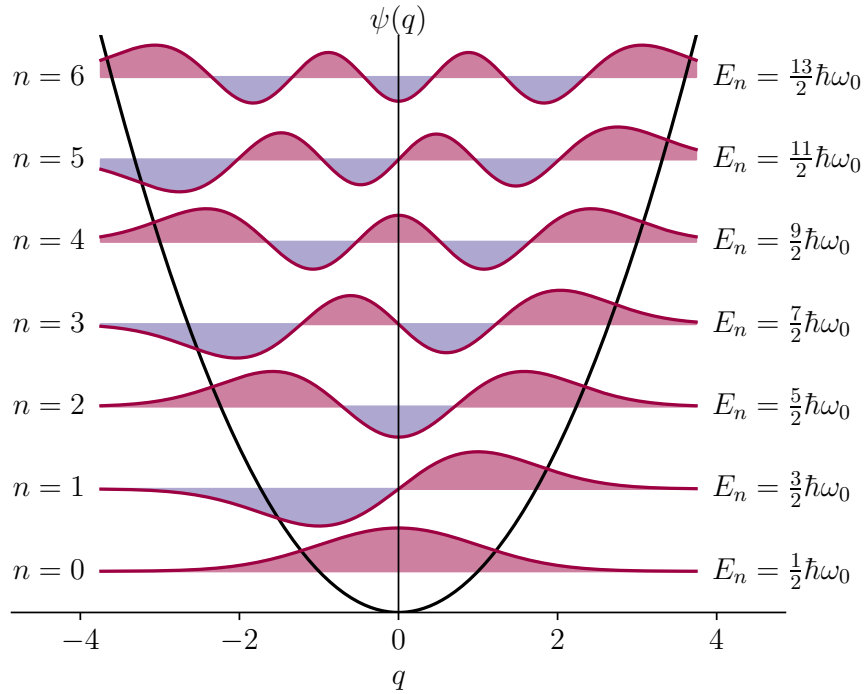
Figure 1: Energy levels $E_n = (n + \frac{1}{2})\hbar\omega_0$ and wave functions for the first six levels of the quantum harmonic oscillator.

Recall that the energy levels of a quantum harmonic oscillator are

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

with $n = 0, 1, 2, \ldots$. A plot of the energy levels and the wave-functions are shown in Fig. 1 below.

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

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

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

$$P_n = Ce^{-E_n/k_BT} = Ce^{-n\hbar\omega_0/k_BT} \tag{11}$$

with C a normalizing constant. $1/C$ is given a symbol Z, which is short for Zustandsumme in German (meaning sum over states). Z is called the partition function in English.

(a) 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 is shown below. Describe qualitatively what this plot is telling you physically.
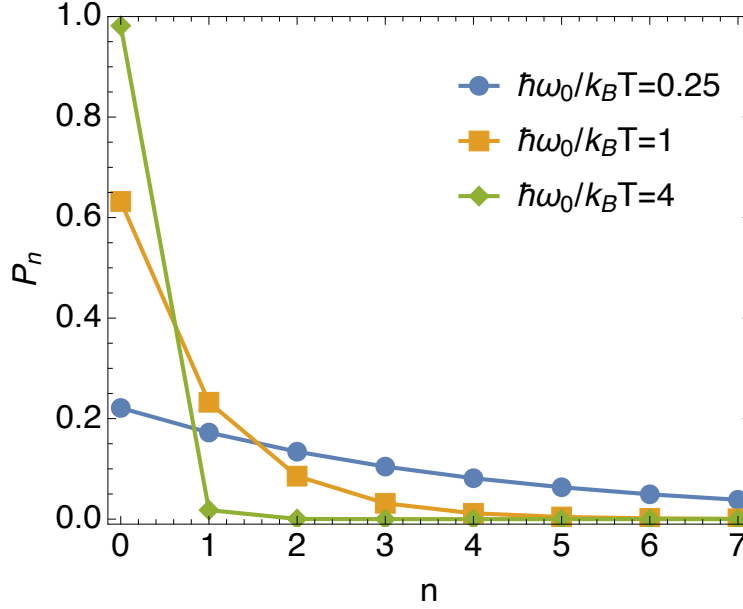
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Figure 2: Probability for the oscillator to have n quanta for different values $\hbar\omega_0/k_B T$.

You should find

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

(c) The first vibrational excited state of diatomic hydrogen H_2 has a spectroscopic wavenum-ber of[2] $1/\lambda_0 = 4400\,\mathrm{cm}^{-1}$. Express the vibrational energy in eV, and give a rough estimate for the temperature when the typical number of vibrational quanta in the vibrations of H_2 becomes of order unity.

Do not use ridiculous constants like $\hbar = 1.05 \times 10^{-34}\,J\,s$ and $k_B = 1.38 \times 10^{-23}\,J/K^{-1}$, but rather try to put it in physical terms: use $\hbar c = 197\,\mathrm{eV\,nm}$, and $k_B T \simeq 1/44\,\mathrm{eV}$ at freezing $273\,^oK$.

Discussion: I find $T \simeq 6000^o$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 1000ºK) they begin to vibrate, and the $\frac{5}{2}k_B T$ 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 1000ºK reflects the vibrational degrees of freedom becoming active

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[2]In spectroscopy one calls wave number $1/\lambda$. In most other branches of physics, wavenumber refers to $k = 2\pi/\lambda$, see here.
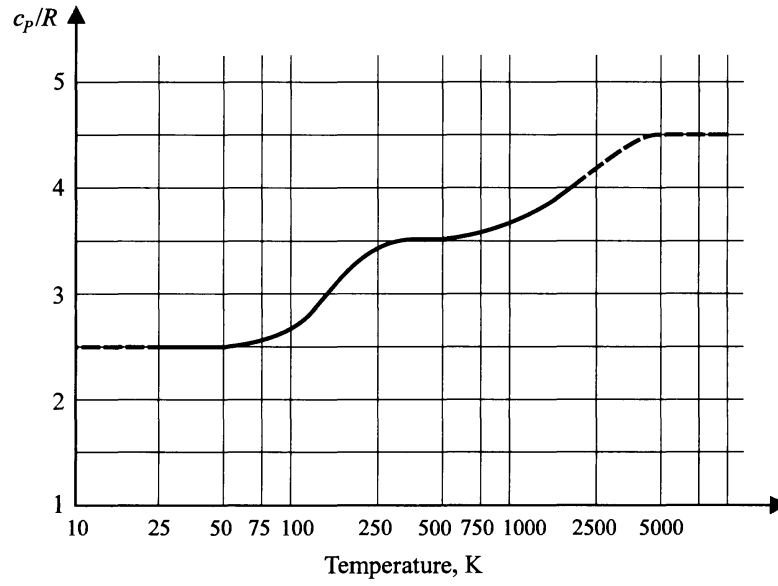
Problem 4.   Probabilities for escaping particles
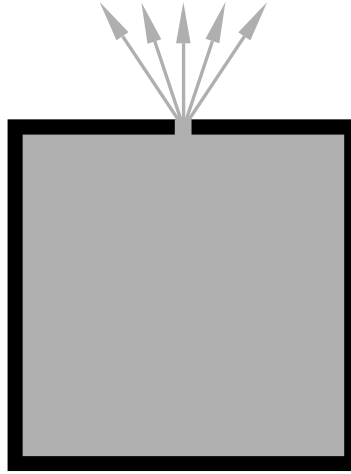
In class we showed the number of particles per area per second passing through a hole in the container with speeds between $(v, v + dv)$, and angles between $(\theta, \theta + d\theta)$ and $(\phi, \phi + d\phi)$ is

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

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.

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(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 $\tau \simeq 1\,\text{hour}$ after being fully inflated. Make an estimate for the area 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 $\tau^{-1} \equiv A(k_B T/2\pi m)^{1/2}/V$ is a characteristic decay time. Thus $A \propto V/\tau (k_B T/m)^{1/2}$

Problem 5.   2D World

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

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

$$\mathrm{d}v_x \mathrm{d}v_y = \left|\left|\frac{\partial(v_x, v_y)}{\partial(v, \theta)}\right|\right| dvd\theta = v\, \mathrm{d}v\, \mathrm{d}\theta \tag{15}$$

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[3]

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

(b) 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

$$\boldsymbol{e}_r \equiv \frac{\partial x}{\partial r}\,\hat{\boldsymbol{\imath}} + \frac{\partial y}{\partial r}\,\hat{\boldsymbol{\jmath}} \tag{17}$$

$$\boldsymbol{e}_\theta \equiv \frac{\partial x}{\partial \theta}\,\hat{\boldsymbol{\imath}} + \frac{\partial y}{\partial \theta}\,\hat{\boldsymbol{\jmath}}. \tag{18}$$

Compute the norms of these vectors $|\boldsymbol{e}_r dr|$ and $|\boldsymbol{e}_\theta d\theta|$ and show that the vectors are orthogonal. Qualitatively interpret these vectors 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.

(c) (Optional. No work) In three dimensions, show that the Jacobian of the map $x = r\sin\theta\cos\phi$, $y = r\sin\theta\cos\phi$, $z = r\cos\theta$, is

$$d^3 x = \left|\left|\frac{\partial(x, y, z)}{\partial(r, \theta, \phi)}\right|\right| drd\theta d\phi = \begin{Vmatrix} \sin\theta\cos\phi & r\cos\theta\cos\phi & -r\sin\theta \\ \sin\theta\sin\phi & r\cos\theta\cos\phi & r\sin\theta \\ \cos\theta & -r\sin\theta & 0 \end{Vmatrix} = r^2 \sin\theta drd\theta d\phi \tag{19}$$
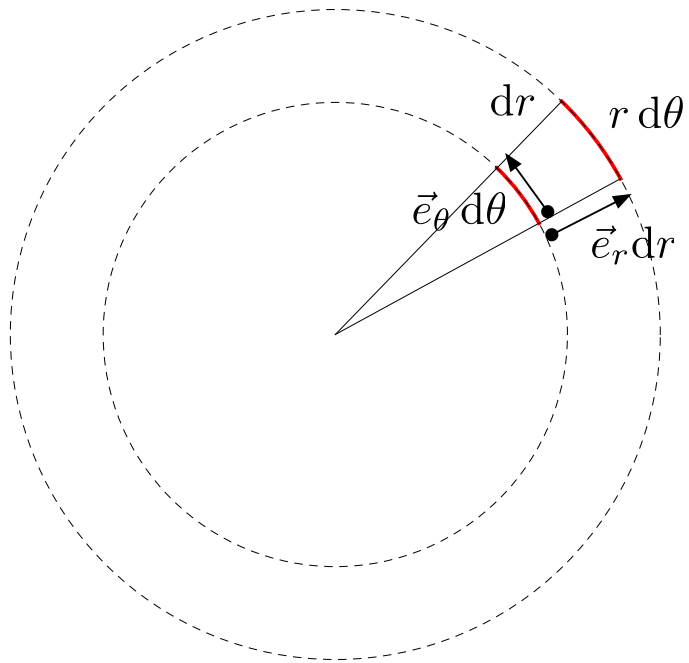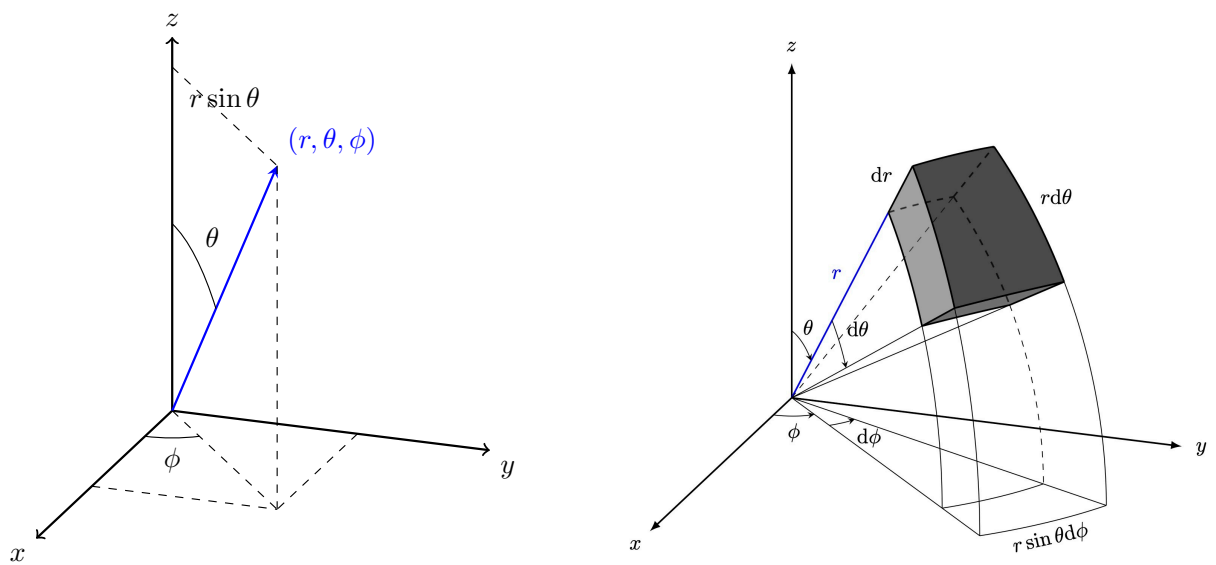
Figure 3: Cylindrical coordinates in two dimensions.

Figure 4: Spherical coordinates.

Look at the columns and find the lengths of $\boldsymbol{e}_r\,dr$, $\boldsymbol{e}_\theta\,d\theta$ and $\boldsymbol{e}_\phi\,d\phi$. Interpret these vectors and lengths by looking at Fig. 4 where the spherical coordinates explained.

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

$$d\mathscr{P}(v) = P(v)dv \tag{20}$$

Describe in plain speak and a simple picture (like Fig. 3) 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 $\left\langle \frac{1}{2}mv^2 \right\rangle$ using the speed distribution. You should find $k_B T$. 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

$$\Phi = \frac{1}{4}n\left\langle v \right\rangle \tag{21}$$

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

$$p = \frac{1}{3}nm\left\langle v^2 \right\rangle \tag{22}$$

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

$$\Phi = \frac{1}{\pi}n\left\langle v \right\rangle \tag{23}$$

$$p = \frac{1}{2}nm\left\langle v^2 \right\rangle \tag{24}$$

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, $\left\langle v \right\rangle = (\pi k_B T/2m)^{1/2}$ and $\left\langle v^2 \right\rangle = 2k_B T/m$, so the results of part (e) establish that:

$$p = nk_B T \tag{25}$$

$$\Phi = \frac{p}{\sqrt{2\pi m k_B T}} \tag{26}$$

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.

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³Sometimes 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.