THE UNIVERSITY OF QUEENSLAND
SCHOOL OF MATHEMATICS AND PHYSICS
PHYS2041 – Quantum Physics

Tutorial 1 Solutions

Problem 1.1 **[FOR ASSIGNMENT 1; max 10 points]**

(a) Use the given distribution and solve for $f(0)$, which is a constant:

$$\begin{aligned} 1 &= \int_{-\infty}^{\infty} f(0) e^{-\frac{x^2}{2\sigma^2}}\, dx \\ &= f(0) \int_{-\infty}^{\infty} e^{-\frac{x^2}{2\sigma^2}}\, dx \end{aligned}$$

Since $e^{-\frac{x^2}{2\sigma^2}}$ is an *even* function, symmetric about the y-axis, we can use the integral given in 1.2 multiplied by 2. Refer to the solution of Problem 1.2 for an in-depth discussion about even and odd functions. So

$$\begin{aligned} 1 &= 2f(0) \int_{0}^{\infty} e^{-ax^2}\, dx \\ &= f(0)\sqrt{\frac{\pi}{a}} \end{aligned}$$

where

$$a = \frac{1}{2\sigma^2}.$$

We then have

$$\begin{aligned} 1 &= f(0)\sqrt{2\pi\sigma^2} \\ f(0) &= \frac{1}{\sqrt{2\pi}\sigma}. \end{aligned}$$

(b) We mentioned before that $f(x)$ is an *even* function. It turns out that $xf(x)$ is an *odd* function – it's anti-symmetric about the y-axis (again, see 1.2 for a more in-depth discussion). This means that the indefinite integral of $xf(x)$ is zero. In other terms,

$$\begin{aligned} \langle x \rangle &= \int_{-\infty}^{\infty} x f(x)\, dx \\ &= 0. \end{aligned}$$

(c) Following our 'even and odd' reasoning from (a) and (b), $x^2 f(x)$ is *even*. This means we can use the appropriate integral in 1.2 and multiply by 2.

$$\begin{aligned}
\langle x^2 \rangle &= \int_{-\infty}^{\infty} x^2 f(x)\ dx \\
&= 2f(0) \int_0^{\infty} e^{-\frac{x^2}{2\sigma^2}}\ dx \\
&= 2f(0) \cdot \frac{1}{4}\sqrt{\pi(2\sigma^2)^3} \\
&= 2 \cdot \frac{1}{\sqrt{2\pi}\sigma} \cdot \frac{1}{4} 2\sqrt{2\pi}\sigma^3 \\
&= \sigma^2.
\end{aligned}$$

(d) Using the definition given,

$$\begin{aligned}
w_{\text{rms}} &= \sqrt{\langle x^2 \rangle - \langle x \rangle} \\
&= \sqrt{\sigma^2 - 0} \\
&= \sigma.
\end{aligned}$$

So, for a Gaussian function in which the exponential part is written down as $\exp(-x^2/2\sigma^2)$**,** σ **is the r.m.s. width, or the actual variance (standard deviation).**

(e) As shown in Figure 1, $f(0)$ is the maximum value of the Gaussian and σ controls the spread.

(f) As shown in (f), the maximum of $f(x)$ is $f(0)$. The width at half of the maximum can be found with

$$\begin{aligned}
f(w_{1/2}) &= \frac{1}{2} f(0) \\
f(0) e^{-\frac{w_{1/2}^2}{2\sigma^2}} &= \frac{1}{2} f(0) \\
e^{-\frac{w_{1/2}^2}{2\sigma^2}} &= \frac{1}{2} \\
-\frac{w_{1/2}^2}{2\sigma^2} &= \ln \frac{1}{2} \\
\frac{w_{1/2}^2}{2\sigma^2} &= \ln 2 \\
w_{1/2} &= \sqrt{2 \ln 2}\, \sigma \\
w_{1/2} &= \sqrt{2 \ln 2}\, w_{\text{rms}}
\end{aligned}$$

Since $\sqrt{2 \ln 2} > 1$, the half-width at half-maximum is larger than the r.m.s. width.

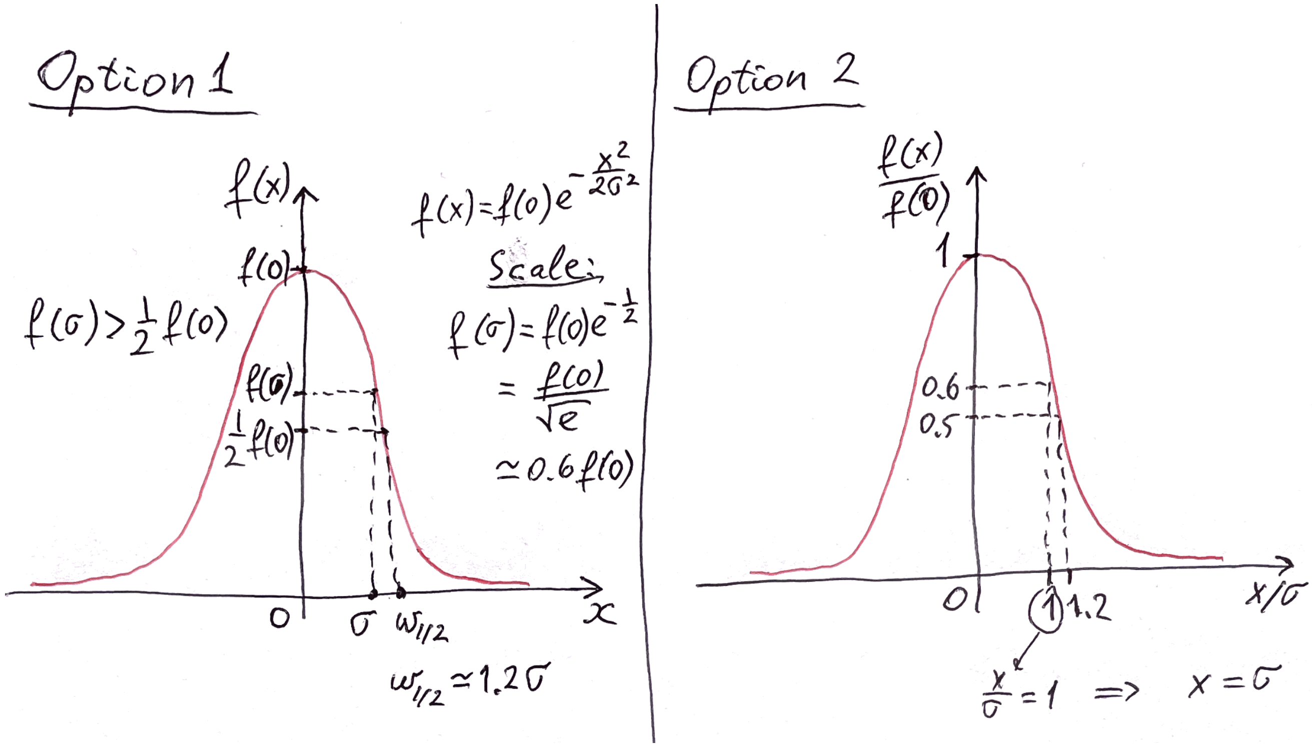

Figure 1: Plot of $f(x)$ illustrating various features of Gaussian distributions.

Problem 1.2

(a) Mathematically speaking the distribution is normalised if $\int d^{(3)}\mathbf{v}P(v_x, v_y, v_z) = 1$, so this is what we need to show. First it is useful to write the integral in terms of its components,

$$\int d^{(3)}\mathbf{v}P(v_x, v_y, v_z) = \left(\frac{m}{2\pi k_B T}\right)^{3/2} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-\frac{m}{2k_BT}\left(v_x^2+v_y^2+v_z^2\right)} dv_x dv_y dv_z \tag{1}$$

$$= \left(\frac{m}{2\pi k_B T}\right)^{3/2} \int_{-\infty}^{\infty} e^{-\frac{m}{2k_BT}v_x^2} dv_x \int_{-\infty}^{\infty} e^{-\frac{m}{2k_BT}v_y^2} dv_y \int_{-\infty}^{\infty} e^{-\frac{m}{2k_BT}v_z^2} dv_z \tag{2}$$

The bottom line follows because the bounds of integration are all constant, and v_x, v_y and v_z are all independent. This is nice to do when you can, because now you can just evaluate each separately.

Before we go any further it'll be useful to briefly discuss odd and even functions, because sometimes we can exploit their properties to simplify integrals. **This will come up throughout the course, so always keep this in the back of your mind!** An even function satisfies $f(-x) = f(x)$ and an odd function satisfies $f(-x) = -f(x)$.

Because $-v^2 = -(-v)^2$ (i.e. $-v^2$ is even), we can deduce that $\exp(-v^2)$ must also be even. This means we can make use of the supplied Gaussian integrals:

$$\int_{-\infty}^{\infty} e^{-\frac{m}{2k_BT}v_x^2} dv_x = \int_{0}^{\infty} e^{-\frac{m}{2k_BT}v_x^2} dv_x + \int_{-\infty}^{0} e^{-\frac{m}{2k_BT}[-v_x]^2} dv_x \tag{3}$$

$$= 2\int_{0}^{\infty} e^{-\frac{m}{2k_BT}v_x^2} dv_x \tag{4}$$

$$= \sqrt{\frac{2\pi k_BT}{m}}, \tag{5}$$

Of course the v_y and v_z integrals are identical, so

$$\int d^{(3)}\mathbf{v}P(v_x, v_y, v_z) = \left(\frac{m}{2\pi k_BT}\right)^{3/2} \left(\frac{2\pi k_BT}{m}\right)^{3/2} = 1, \tag{6}$$

as required.

(b) The mean of any quantity $f(x)$ with respect to the distribution $P(x)$ is $\langle f(x)\rangle = \int_{-\infty}^{\infty} f(x)P(x)dx$. So our task is to evaluate

$$\langle v_x\rangle = \left(\frac{m}{2\pi k_BT}\right)^{3/2} \int_{-\infty}^{\infty} v_x e^{-\frac{m}{2k_BT}v_x^2} dv_x \int_{-\infty}^{\infty} e^{-\frac{m}{2k_BT}v_y^2} dv_y \int_{-\infty}^{\infty} e^{-\frac{m}{2k_BT}v_z^2} dv_z, \tag{7}$$

and also the corresponding integrals for $\langle v_y\rangle$ and $\langle v_z\rangle$.

Before we blindly charge ahead let's stop and think. In the previous question we deduced that $\exp(-v^2)$ is an even function. Clearly v is odd, which means $v\exp(-v^2)$ must also be odd. This is easy to see since: $(-v)\exp(-[-v]^2) = -v\exp(-v^2)$. This means the integral goes to 0:

$$\int_{-\infty}^{\infty} v_x e^{-\frac{m}{2k_BT}v_x^2} dv_x = \int_{0}^{\infty} v_x e^{-\frac{m}{2k_BT}v_x^2} dv_x + \int_{-\infty}^{0} (-v_x) e^{-\frac{m}{2k_BT}v_x^2} dv_x \tag{8}$$

$$= \int_{0}^{\infty} v_x e^{-\frac{m}{2k_BT}v_x^2} dv_x - \int_{0}^{\infty} v_x e^{-\frac{m}{2k_BT}v_x^2} dv_x \tag{9}$$

$$= 0 \tag{10}$$

In fact, this is true for any odd function. Thus we can deduce, (without having to actually do any integrals!) that $\langle v_x\rangle = \langle v_y\rangle = \langle v_z\rangle = 0$ and so,

$$\langle \mathbf{v}\rangle = (0, 0, 0). \tag{11}$$

This answer makes sense for a couple of reasons. Once you've had some experience looking at Gaussians you should be able to spot that the distribution Eq.(1) is centred around 0, i.e. the mean is 0. Physically it makes sense too, according to the kinetic theory of gasses we picture a hot gas as a collection of independent particles vibrating and moving around randomly, so we would expect the velocity to average to 0 (in the absence of any external forces acting on the particles, of course).

(c) The procedure to find $\langle v^2 \rangle = \langle |\mathbf{v}|^2 \rangle = \langle v_x^2 \rangle + \langle v_y^2 \rangle + \langle v_z^2 \rangle$ is the same as in the part (**b**), except the integral we need to evaluate is now

$$\langle v_x^2 \rangle = \left(\frac{m}{2\pi k_B T} \right)^{3/2} \int_{-\infty}^{\infty} v_x^2 e^{-\frac{m}{2k_B T} v_x^2} dv_x \int_{-\infty}^{\infty} e^{-\frac{m}{2k_B T} v_y^2} dv_y \int_{-\infty}^{\infty} e^{-\frac{m}{2k_B T} v_z^2} dv_z \tag{12}$$

and also the corresponding integrals for $\langle v_y^2 \rangle$ and $\langle v_z^2 \rangle$.

Unfortunately (or fortunately, if you love doing Gaussian integrals!), $v^2 \exp(-v^2)$ is *even* so the integral won't vanish this time. But as with part (**a**) we can use this fact to simplify the integral, and then use the provided Gaussian integrals (Eq. (3) in the list of integrals with $n = 1$) to find:

$$\begin{aligned} \int_{-\infty}^{\infty} v_x^2 e^{-\frac{m}{2k_B T} v_x^2} dv_x &= 2 \int_{0}^{\infty} v_x^2 e^{-\frac{m}{2k_B T} v_x^2} dv_x & (13) \\ &= \frac{1}{2} \sqrt{\frac{\pi (2k_B T)^3}{m^3}}. & (14) \end{aligned}$$

Using this result, combined with the integrals we used in part (**a**) gives

$$\begin{aligned} \langle v_x^2 \rangle &= \left(\frac{m}{2\pi k_B T} \right)^{3/2} \frac{1}{2} \sqrt{\frac{\pi (2k_B T)^3}{m^3}} \sqrt{\frac{2\pi k_B T}{m}} \sqrt{\frac{2\pi k_B T}{m}} & (15) \\ &= \frac{k_B T}{m}. & (16) \end{aligned}$$

Following similar reasoning it's easy to deduce that $\langle v_y^2 \rangle = \langle v_z^2 \rangle = k_B T/m$ also. Therefore the expectation value of the total velocity squared is

$$\begin{aligned} \langle v^2 \rangle = \langle |\mathbf{v}|^2 \rangle &= \langle v_x^2 \rangle + \langle v_y^2 \rangle + \langle v_z^2 \rangle & (17) \\ &= \frac{3k_B T}{m} & (18) \end{aligned}$$

This result merits a brief discussion. You may recall from thermodynamics that the mean kinetic energy obeys the equipartition theorem which states for a monatomic gas (i.e., with three motional degrees of freedom, simply the kinetic energy along the x,y and z directions) the mean kinetic energy per particle obeys "$\frac{1}{2} k_B T$" times "No. of degrees of freedom", i.e.:

$$\langle E_{kin} \rangle = \frac{1}{2} m \langle v^2 \rangle = \frac{3}{2} k_B T, \tag{19}$$

which is exactly the result we just derived! Do not fall into the trap of assuming that a quantity with zero mean also has zero mean square, this is rarely the case! The mean square is a useful measure of the *spread* in some quantity.

(d) **Brief overview of spherical coordinates.**
Spherical coordinates may seem confusing, but as we'll see here they can actually make our lives

much easier. If you're not familiar with spherical coordinates the wiki article is a good summary `https://en.wikipedia.org/wiki/Spherical_coordinate_system`. Briefly, we introduce new coordinates r, θ and φ which are related to the Cartesian x,y,z coordinates by,

$$x = r\sin\theta\cos\varphi \tag{20}$$
$$y = r\sin\theta\sin\varphi \tag{21}$$
$$z = r\cos\theta \tag{22}$$

with radius $0 \leq r = \sqrt{x^2+y^2+z^2} < \infty$, azimuthal angle $0 \leq \varphi \leq 2\pi$ and elevation angle $0 \leq \theta \leq \pi$. **Be warned, mathematicians tend to swap the definitions of θ and φ.** The definition I've used here follows the textbook, and is commonly used by physicists. But be wary, courses such as MATH2000/MATH2001 may use a different convention.

Integrals also look a little different in spherical coordinates,

$$\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz f(x,y,z) = \int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta\, d\theta \int_0^{\infty} dr\, r^2\, f(r,\varphi,\theta) \tag{23}$$

The factor of $r^2\sin\theta$ is called the *Jacobian*, it arises as a result of transforming a cubic volume element to a spherical one. Also, without it the units would be inconsistent. Let's get into the question now.

Normalisation integral.
For a velocity distribution the Cartesian coordinates are v_x, v_y and v_z, and so $v^2 = v_x^2 + v_y^2 + v_z^2 = r^2$, (i.e. our "radius" actually has dimensions of velocity). This is the advantage of spherical coordinates, the distribution P is a function of r only, rather than three Cartesian coordinates. The normalisation integral becomes

$$\int d^{(3)}\mathbf{v} P(v_x,v_y,v_z) = \tag{24}$$

$$= \left(\frac{m}{2\pi k_B T}\right)^{3/2} \underbrace{\int_0^{2\pi} d\varphi}_{=2\pi} \underbrace{\int_0^{\pi} \sin\theta d\theta}_{=2} \int_0^{\infty} e^{-\frac{m}{2k_BT}r^2} r^2 dr \tag{25}$$

To evaluate the radial integral we can just use the same Gaussian integral as part (**c**),

$$\int_0^{\infty} e^{-\frac{m}{2k_BT}r^2} r^2 dr = \frac{1}{4}\sqrt{\frac{\pi(2k_BT)^3}{m^3}}. \tag{26}$$

Putting this back into the normalisation integral gives

$$\int d^{(3)}\mathbf{v} P(v_x,v_y,v_z) = \left(\frac{m}{2\pi k_B T}\right)^{3/2} \left(\frac{1}{4}\sqrt{\frac{\pi(2k_BT)^3}{m^3}}\right) 4\pi = 1, \tag{27}$$

as required.

Mean square integral.
The integral for $\langle v^2\rangle$ is now (using $\int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta d\theta = 4\pi$):

$$\langle v^2\rangle = 4\pi \left(\frac{m}{2\pi k_B T}\right)^{3/2} \int_0^{\infty} r^4 e^{-\frac{m}{2k_BT}r^2} dr. \tag{28}$$

Notice that spherical coordinates reduce this calculation to a single integral, rather than three integrals for $\langle v_x^2\rangle$, $\langle v_y^2\rangle$ and $\langle v_z^2\rangle$. The factor of r^4 comes from two factors of r^2, one from the Jacobian and one because we're calculating $\langle v^2\rangle$. Using the provided Gaussian integrals (Eq. (3) in the list of integrals with $n=2$),

$$\int_0^\infty r^4 e^{-\frac{m}{2k_BT}r^2}dr = \frac{3}{8}\sqrt{\frac{\pi(2k_BT)^5}{m^5}} = \frac{3\sqrt{\pi}}{8}\left(\frac{2k_BT}{m}\right)^{5/2} \tag{29}$$

which gives

$$\langle v^2\rangle = 4\pi\left(\frac{m}{2\pi k_BT}\right)^{3/2}\frac{3\sqrt{\pi}}{8}\left(\frac{2k_BT}{m}\right)^{5/2} = \frac{3k_BT}{m}, \tag{30}$$

as required.

Problem 1.3 [FOR ASSIGNMENT 1; max 10 points]

(a)

$$Z = \sum_{n=0}^{\infty} e^{-nx} = \sum_{n=0}^{\infty}(e^{-x})^n = \sum_{n=0}^{\infty} q^n, \tag{31}$$

where we have defined $q \equiv e^{-x}$. For $x > 0$ we have a geometric series, which converges for $|q| < 1$. Hence,

$$Z = \sum_{n=0}^{\infty} q^n = \frac{1}{1-q} = \frac{1}{1-e^{-x}} \tag{32}$$

(b)

$$Z' = \int_0^\infty \mathrm{d}n\, e^{-nx} = \frac{1}{x}\int_0^\infty \mathrm{d}y e^{-y} = \frac{1}{x}(-e^{-y})\Big|_0^\infty = \frac{1}{x}(0+1) = \frac{1}{x}, \tag{33}$$

where we have used the substituion $y \equiv nx$ and $\mathrm{d}n = \mathrm{d}y\, 1/x$.

(c)

Using the Taylor expansion where $e^{-x} = 1 - x + x^2/2 + \ldots$,

$$Z = \frac{1}{1-(1-x+\ldots)} = \frac{1}{x} = Z'. \tag{34}$$

Here we assumed that all orders higher than the linear term vanish because $x \ll 1$. For a black-body radiator, we associate $x \equiv \hbar\omega/k_BT$, where ω is the frequency of the E.M. radiation, T is the temperature, and k_B and $\hbar$ are the usual Boltzmann and Planck constants. We further identify that Z and Z' are the partition functions for a single mode of E.M. radiation.

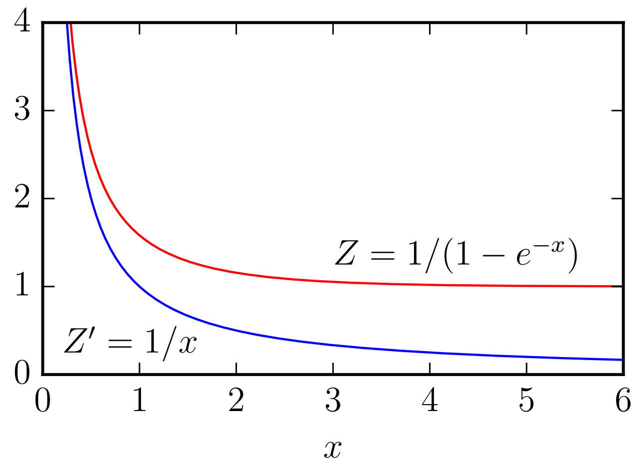

Figure 2: Comparison between discrete and continous variables. Note that Z, Z', $x > 0$. The domain is chosen to capture the interesting features of the plot, it's unwise to plot for values of x much larger than this because it obscures interesting details for $x < 1$!

In the classical regime we can treat the E.M. radiation as continuous, while in the quantum regime Planck's result tells us that E.M. radiation can only be emitted in discrete packets (i.e., photons). The result above tells us that for $\hbar\omega/k_BT \ll 1$, our quantum partition function (the discrete case Z) recovers the classical result given by Z'. Therefore, we identify the "classical" regime for a black-body radiator when $\hbar\omega/k_BT \ll 1$ (e.g., at very large T).