Assignment 1 45855201

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

Properties of a Gaussian function.

Consider the probability distribution function for a quantity x given by a Gaussian function

$$f(x) = f(0)e^{-x^2/(2\sigma^2)}.$$

(a) What should be the value of $f(0)$ so that the distribution function is normalised to unity, $\int_{-\infty}^{+\infty} dx f(x) = 1$?

Evaluate the integral:

$$1 = \int_{-\infty}^{\infty} dx\ f(x) = \int_{-\infty}^{\infty} dx\ f(0)\, e^{-x^2/(2\sigma^2)}$$ (This is an even function, $\int_{-\infty}^{\infty}$ even func $= 2\int_0^{\infty}$ even func)

$$1 = f(0) 2\int_0^{\infty} e^{-x^2/(2\sigma^2)}$$

$$1 = 2f(0) \times \tfrac{1}{2}\sqrt{\pi/\tfrac{1}{2\sigma^2}}$$ $\int_0^{\infty} e^{-ax^2} = \frac{1}{2}\sqrt{\pi/a}$

$$1 = f(0)\sqrt{\pi 2\sigma^2}$$

$$f(0) = (2\pi\sigma^2)^{-1/2}$$

(b) What is the average value of the quantity x, $\langle x \rangle = \int_{-\infty}^{+\infty} dx\, x\, f(x)$?

$$\langle x \rangle = \int_{-\infty}^{\infty} dx\ x \times (2\pi\sigma^2)^{-1/2} e^{-x^2/2\sigma^2}$$

$$= (2\pi\sigma^2)^{-1/2}\int_{-\infty}^{\infty} dx\, x\, e^{-x^2/2\sigma^2}$$ this is an odd function, $\int_{-\infty}^{\infty}$ odd func $= 0$

$$\langle x \rangle = 0$$

(c) What is the average value of x^2, $\langle x^2 \rangle = \int_{-\infty}^{+\infty} dx\, x^2\, f(x)$.

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} dx\ x^2\, (2\pi\sigma^2)^{-1/2} e^{-x^2/2\sigma^2}$$

$$= (2\pi\sigma^2)^{-1/2} \times 2\int_0^{\infty} dx\, x^2 e^{-x^2/2\sigma^2}$$ (this is an even func)

$$= (2\pi\sigma^2)^{-1/2} \times 2 \times \tfrac{1}{4}\sqrt{\pi/(1/2\sigma^2)^3}$$ $\int_0^{\infty} x^2 e^{-ax^2} dx = \frac{1}{4}\sqrt{\pi/a^3}$

$$= \tfrac{1}{2}\sqrt{8\pi\sigma^6 / 2\pi\sigma^2}$$

$$= \tfrac{1}{2}\sqrt{4\sigma^4}$$

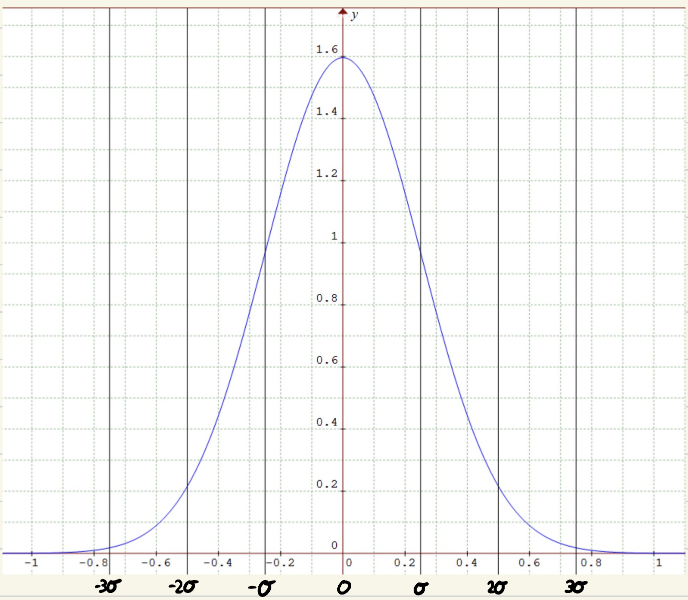
$$= \sigma^2$$

(d) Define the r.m.s (root mean square) width of the distribution function $f(x)$ as $w_{\rm rms} = \sqrt{\langle x^2\rangle - \langle x\rangle^2}$. Find $w_{\rm rms}$ for the above $f(x)$. What is the meaning of σ in the above Gaussian $f(x)$?

$$w_{rms} = \sqrt{\langle x^2\rangle - \langle x\rangle^2}$$
$$= \sqrt{\sigma^2 - 0}$$ from part b) & c)
$$w_{rms} = \sigma$$ rms is a +ive quantity, ignore -ive root solution

σ is the standard deviation of $f(x)$, a number which quantifies the spread of the data around the data's mean.

(e) Plot the function $f(x)$ on a computer for the values $f(0)$ and σ of your choice or sketch $f(x)$ by hand, but indicate the main properties on the graph; in particular, indicate on the graph the length scale on the x axis corresponding to σ.



$$\sigma = 0.25$$
$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-x^2/2\sigma^2}$$
$$= \frac{1}{\sqrt{2\pi \times 1/16}} e^{-x^2/2\times 1/16}$$
$$f(x) = \frac{1}{\sqrt{\pi/8}} e^{-8x^2} \cong 1.6 e^{-8x^2}$$

(f) Find the half-width at half-maximum of $f(x)$ (define it as $w_{1/2}$) and compare it with w_{rms}; which one is larger?

I am assuming that this question is asking to find the tive x value when this function is half of it's maximum

$f(x) = 1/\sqrt{2\pi\sigma^2} \times e^{-x^2/2\sigma^2}$ The maximum value of this function occurs when $x=0$ (graph in e). Therfore max $= 1/\sqrt{2\pi\sigma^2}$ and half-max $= 1/2\sqrt{2\pi\sigma^2}$

solve for $x \rightarrow$

$$\frac{1}{2\sqrt{2\pi\sigma^2}} = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-x^2/2\sigma^2}$$

$$1/2 = e^{-x^2/2\sigma^2}$$

$$\ln(1/2) = \ln(e^{-x^2/2\sigma^2})$$

$$-\ln(2) = -x^2/2\sigma^2$$

$$x^2 = \ln(2) \times 2\sigma^2$$

$$x = \sqrt{\ln(2) \times 2 \times \sigma^2}$$

$$x = \sigma \times \sqrt{\ln(4)}$$

$$x \approxeq 1.18\sigma$$

The half-width is approximatley 1.18 times larger than the w_{rms}

Problem 1.3 **[FOR ASSIGNMENT 1; max 10 points]**

Discrete versus continuous variables ('quantum' versus 'classical').

This problem is a simple illustration of how an infinite series involving discrete (read 'quantised', in the context of quantum mechanics) variables can lead to a very different result compared to a similar integration over a continuous variable.

(a) Evaluate the following infinite series:

$$Z = \sum_{n=0}^{\infty} e^{-nx}, \ (n = 0, 1, 2, 3, ...), \tag{2}$$

clearly stating and checking the condition for its convergence.

$Z = \sum_{n=0}^{\infty} e^{-nx}, \quad n = 0, 1, 2, 3, 4$

$Z = 1 + e^{-x} + e^{-2x} + e^{-3x} + e^{-4x} ...$

$Z = 1 + e^{-x}(1 + e^{-x} + e^{-2x} + e^{-3x} ....)$

$Z = 1 + Z \times e^{-x}$

$1 = Z - Ze^{-x}$

$1 = Z(1 - e^{-x})$

$Z = \dfrac{1}{1 - e^{-x}} \quad x \neq 0$

Checking for ROC

$e^{-nx} < 1, \quad n = 0, 1, 2, 3 ...$

$-nx < 0$

$-x < 0$

$x > 0$

$\therefore$ For the series to converge $x > 0$

(b) Now evaluate the following integral:

$$Z' = \int_0^{\infty} e^{-nx} dn. \tag{3}$$

Note that the integration is not over x, but over n, which is assumed to be real and nonnegative.

[According to the definition of a definite integral, $\int_0^{\infty} e^{-nx} dn = \lim_{\Delta n \to 0} \sum_{i=0}^{\infty} e^{-n_i x} \Delta n$, with $n_0 = 0, n_1 = \Delta n, n_2 = 2\Delta n, ..., n_i = i\Delta n, ...$. If the characteristic decay 'length' of the exponential function (determined by the value of $1/x$, with the exponential 'function' being a function of n, while x being treated as a parameter) was much larger than unity, one could evaluate the integral numerically using $\Delta n = 1$ as a good approximation, in which case the resulting infinite series would be equivalent to Z.]

$$Z' = \int_0^\infty e^{-nx}\, dn$$
$$= \left[\frac{1}{-x} e^{-nx}\right]_0^\infty$$
$$= \left[\lim_{n\to\infty}\left(\frac{1}{-x} e^{-nx}\right) - \frac{1}{-x} e^{-0\times x}\right]$$
$$= 0 - \frac{1}{-x} e^0$$
$$Z' = \frac{1}{x}$$

(c) Plot the results for Z and Z' on the same graph (using, e.g., Matlab) as functions of x. In the context of the spectrum of black-body radiation, the quantity x corresponds to $x \equiv \hbar\omega/k_B T$, where ω is the frequency of the E.M radiation and T is the temperature; the quantity Z in quantum statistical mechanics refers to the partition function of a single mode of E.M. radiation at frequency ω. Next simplify the resulting expression for Z, for $x \ll 1$, using Taylor expansion. What do you conclude form this expansion and comparison to Z'?

Taylor series with centre 0

$$e^{-x} = \sum_{n=0}^{\infty} (-1)^n \frac{x^n}{n!}$$
$$= 1 - x + \frac{1}{2}x^2 - \frac{1}{6}x^3 + \frac{1}{24}x^4$$

$$\therefore Z \approxeq \frac{1}{1-(1-x+\frac{1}{2}x^2+\dots)}$$

when $x \ll 1$, x is the most significant term $\therefore$

at $x \ll 1$ $\quad Z \approxeq \dfrac{1}{1-(1-x)}$

$$Z \approxeq \frac{1}{x}$$

$\therefore$ when $x \ll 1$ $\quad Z \approxeq Z'$

Problem 2.2 **[FOR ASSIGNMENT 1; max 10 points]**

Suppose we add a constant V_0 to the potential energy V. [By "constant" we mean independent of x and t.] In *classical* mechanics, where the Newton's law reads as

$$m\frac{d^2x}{dt^2} = -\frac{\partial V}{\partial x}, \tag{1}$$

this doesn't change anything, but what about *quantum* mechanics? Show that the wave function picks up a time dependent phase factor $\exp(-iV_0t/\hbar)$, *i.e.*, the wave function (Ψ_0) with V_0 added relates to the wave function (Ψ) without V_0 as:

$$\Psi_0 = \Psi e^{-iV_0t/\hbar}.$$

What effect does this have on the expectation value of a dynamical quantity? Explain why.

assume Ψ_0 satisfies the wave equation

$$i\hbar\frac{\partial\Psi_0}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi_0}{\partial x^2} + (V(x,t)+V_0)\Psi_0$$

sub $\Psi_0 = \Psi e^{-iV_0t/\hbar} \rightarrow$ $$i\hbar\frac{\partial}{\partial t}\left(\Psi e^{-iV_0t/\hbar}\right) = -\frac{\hbar^2}{2m}e^{-iV_0t/\hbar}\frac{\partial^2\Psi}{\partial x^2} + (V(x,t)+V_0)\Psi e^{-iV_0t/\hbar}$$

apply product rule $\rightarrow$ $$i\hbar\left(\Psi \times \frac{-iV_0}{\hbar}\times e^{-iV_0t/\hbar} + \frac{\partial(\Psi)}{\partial t}e^{-iV_0t/\hbar}\right) = -\frac{\hbar^2}{2m}e^{-iV_0t/\hbar}\frac{\partial^2\Psi}{\partial x^2} + (V(x,t)+V_0)\Psi e^{-iV_0t/\hbar}$$

$$e^{-iV_0t/\hbar}\left(\Psi V_0 + i\hbar\frac{\partial}{\partial t}(\Psi)\right) = e^{-iV_0t/\hbar}\left(\frac{-\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + (V(x,t)+V_0)\Psi\right)$$

$$\Psi V_0 + i\hbar\frac{\partial\Psi}{\partial t} = \frac{-\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x,t)\Psi + V_0\Psi$$

$$i\hbar\frac{\partial\Psi}{\partial t} = \frac{-\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x,t)\Psi$$

$\therefore$ the constant only adds a time dependant phase factor

This has no effect on the expectation values:

$$\langle x\rangle = \int_{-\infty}^{\infty} dx\, x\, |\Psi_0(x,t)|^2 = \int_{-\infty}^{\infty} dx\,(\Psi_0^* x \Psi_0) = \int_{-\infty}^{\infty} dx\,(\Psi^* e^{iV_0t/\hbar}\, x\, \Psi e^{-iV_0t/\hbar})$$
$$= \int_{-\infty}^{\infty} dx\,(\Psi^* x \Psi)$$

Given some particle with some distribution of position & momentum distributions. Adding a constant potential to this particle independant of time and position, doesn't effect the position & momentum distribution.

Problem 2.3 **[FOR ASSIGNMENT 1; max 10 points]**

Consider a particle described by the wave function

$$\Psi(x,t) = Ce^{-i\omega t}e^{-b|x|}, \tag{2}$$

where C and b are real and positive constants.

(a) Normalise the wave function, i.e., find C (in terms of b) such that the wave function is normalised to unity. Recall that

$$|x| = \begin{cases} x, & \text{for } x \geq 0, \\ -x, & \text{for } x < 0. \end{cases} \tag{3}$$

(b) Calculate the expectation values of x and x^2.

(c) Determine the standard deviation (σ_x) of x. Plot (using , e.g., Matlab) or sketch the graph of $|\Psi|^2$ as a function of x, and mark the points ($\langle x\rangle + \sigma_x$) and ($\langle x\rangle - \sigma_x$), as well as the respective values of $|\Psi|^2$, to illustrate the sense in which σ_x represents the "spread" in x. Show the peak value of $|\Psi|^2$ (in terms of b) on the vertical axis, which will then indicate the respective scale. Also mark (approximately, if you are sketching by hand) the points corresponding to $x = \pm 1/b$ and the respective value of $|\Psi|^2$.

(d) What is the probability that the particle would be found *outside* the range $\langle x\rangle - \sigma_x < x < \langle x\rangle + \sigma_x$?

(e) Determine the probability that the particle would be found *inside* this range, without evaluating the respective integrals again.

a) $\Psi(x,t) = Ce^{-i\omega t}e^{-b|x|}$

A normalised wave function follows this equation

$1 = \int_{-\infty}^{\infty} dx \, |\Psi(x,t)|^2$ at $t=0$

$= \int_{-\infty}^{\infty} dx \, \Psi^*\Psi$

$= \int_{-\infty}^{\infty} dx \, Ce^{i\omega t}e^{-b|x|} \times Ce^{-i\omega t}e^{-b|x|}$

This is an even function: $1 = 2\int_0^{\infty} dx \, C^2 e^{-2bx}$

$= 2C^2 \left[\frac{1}{-2b} e^{-2bx}\right]_0^{\infty}$

$1 = 2C^2\left(\frac{1}{2b}\right)$

$C = \sqrt{b}$ $\qquad \therefore \Psi(x,t) = \sqrt{b}\,e^{-i\omega t}e^{-b|x|}$

b) $\langle x\rangle = \int_{-\infty}^{\infty} dx \, x \, |\Psi(x,t)|^2$

$= \int_{-\infty}^{\infty} dx \, x \, (\Psi(x,t) \times \Psi(x,t)^*)$

$= \int_{-\infty}^{\infty} dx \, x \left(\sqrt{b}\,e^{-b|x|}e^{-i\omega t} \times \sqrt{b}\,e^{-b|x|}e^{i\omega t}\right)$

$= \int_{-\infty}^{\infty} dx \, x \left(b\,e^{-2b|x|} \times e^{0}\right)$

$= \int_{-\infty}^{\infty} dx \, x \left(b e^{-2b|x|}\right)$

$$= b\int_{-\infty}^{\infty} dx \; x e^{-b|x|}$$

This is an odd function $\therefore$ the integral equals zero

$$\langle x \rangle = 0$$

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} dx \; x^2 |\Psi(x,t)|^2$$

$$= \int_{-\infty}^{\infty} dx \; x^2 \left(\Psi(x,t) \times \Psi(x,t)^*\right)$$

$$= \int_{-\infty}^{\infty} dx \; x^2 \left(\sqrt{b}\, e^{-b|x|} e^{-i\omega t} \times \sqrt{b}\, e^{-b|x|} e^{i\omega t}\right)$$

$$= \int_{-\infty}^{\infty} dx \; x^2 \left(b\, e^{-2b|x|} \times e^{0}\right)$$

$$= \int_{-\infty}^{\infty} dx \; x^2 \left(b\, e^{-2b|x|}\right)$$

$$= b\int_{-\infty}^{\infty} dx \; x^2 e^{-2b|x|}$$

This is an even function

$$\therefore \quad = 2b \int_{0}^{\infty} dx \; x^2 e^{-2bx} \qquad \int_0^\infty x^2 e^{-ax} = 2/a^3$$

$$= 2b \times \left(1/4b^3\right)$$

$$\langle x^2 \rangle = \frac{1}{2b^2}$$

c) $\sigma_x = ?$

$$\sigma_x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$$

$$= \sqrt{\frac{1}{2b^2} - 0}$$

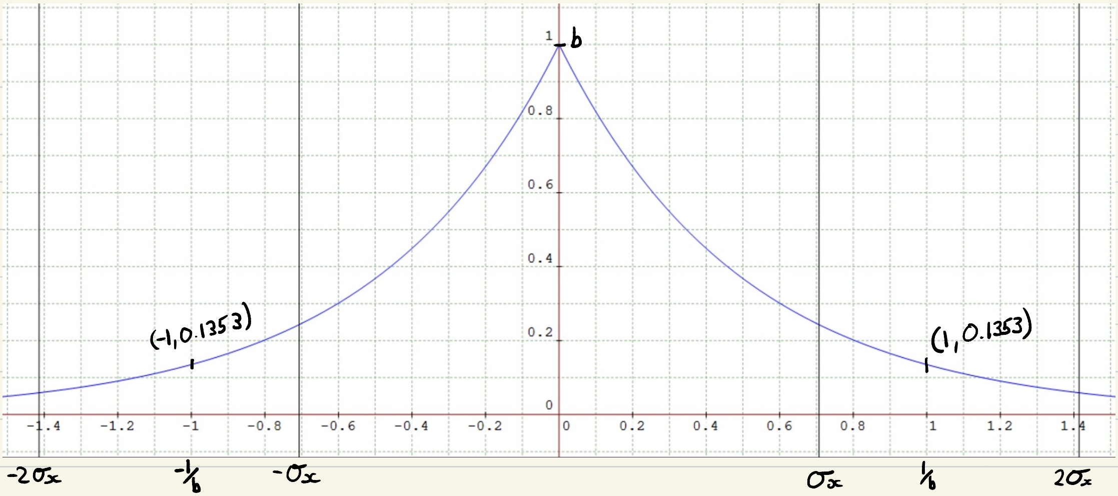
$$\sigma_x = (2b^2)^{-1/2}$$

$$|\Psi|^2 = \Psi^* \Psi$$

$$= \sqrt{b}\, e^{-b|x|} e^{-i\omega t} \times \sqrt{b}\, e^{-b|x|} e^{i\omega t}$$

$$= b\, e^{-2b|x|}$$

plot $|\psi^2|$ when $b=1$ $\quad y = e^{-2|x|}$ $\quad \sigma_x = (2)^{-\frac{1}{2}}$



d) The area outside of one standard deviation is one minus the area inside one standard deviation

$$= 1 - \int_{-\sigma_x}^{\sigma_x} |\Psi(x,t)|^2 \, dx$$

$$= 1 - \int_{-\sigma_x}^{\sigma_x} b\, e^{-2b|x|} \, dx$$

$$= 1 - 2\int_0^{\sigma_x} b\, e^{-2bx} \, dx$$

$$= 1 - 2b \times \frac{1}{-2b} \left[e^{-2bx}\right]_0^{\sigma_x}$$

$$= 1 + \left(e^{-2b\sigma_x} - 1\right)$$

$$= 1 + \left(e^{-2b\frac{1}{\sqrt{2b^2}}} - 1\right)$$

$$= e^{-2\left(b^2/2b^2\right)^{\frac{1}{2}}}$$

$$= e^{-\sqrt{2}} \cong 0.2431$$

e) The area inside one standard deviation is one minus the area outside (value from d)

$$= 1 - e^{-\sqrt{2}}$$

$$\cong 0.7569$$