NTNU – Trondheim
Norwegian University of
Science and Technology

NTNU, Department of Physics

FY2045 Mandatory problem set fall 2023

Henning G. Hugdal

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Problem 1

a) Since the Gaussian probability density $|\psi(x)|^2 = \sqrt{\frac{2\beta}{\pi}} \exp[-2\beta(x-a)^2]$ is symmetric about the point $x = a$, we have $\underline{\underline{\langle x \rangle = a}}$.

b) The uncertainty is defined as the *root-mean-square deviation* (rms dev.). The resulting integral can be calculated using one of the formulas for the Gaussian integrals (with $y = x - a$):

$$\begin{aligned}
(\Delta x)^2 &= \langle (x - \langle x \rangle)^2 \rangle = \langle (x-a)^2 \rangle \\
&= \sqrt{\frac{2\beta}{\pi}} \int_{-\infty}^{\infty} (x-a)^2 e^{-2\beta(x-a)^2} dx = \sqrt{\frac{2\beta}{\pi}} \int_{-\infty}^{\infty} y^2 e^{-2\beta y^2} dy \\
&= \sqrt{\frac{2\beta}{\pi}} \frac{1}{2} \sqrt{\pi} (2\beta)^{-3/2} = \underline{\underline{\frac{1}{4\beta}}}. \qquad (1)
\end{aligned}$$

This means that we can get an arbitrarily small uncertainty, $\Delta x = \frac{1}{2\sqrt{\beta}}$, by choosing a sufficiently large β. With $(\Delta x)^2 = 1/(4\beta)$, i.e., $\beta = 1/[4(\Delta x)^2]$, this Gaussian probability distribution may be expressed as

$$\underline{\underline{|\psi(x)|^2 = \frac{1}{\sqrt{2\pi(\Delta x)^2}} \exp\left[-\frac{(x-a)^2}{2(\Delta x)^2}\right]}}. \qquad (2)$$

Moral: For a Gaussian probability density of this type, we can read off the uncertainty from the exponent. An example: A probability density of the form $|\psi(x)|^2 \propto \exp[-(x-b)^2/c]$ corresponds to an uncertainty determined by the relation $c = 2(\Delta x)^2$.

c) For a *real-valued* wavefunction $\psi(x)$ we see that the expectation value $\langle p_x \rangle = \int \psi \frac{\hbar}{i} \frac{\partial}{\partial x} \psi \, dx = -i\hbar \int \psi \frac{\partial \psi}{\partial x} \, dx$ must be equal to zero; otherwise it would be *purely imaginary* according to the expression above. (Remember that Hermitian operators have real expectation values.) We can also show this explicitly:

$$\begin{aligned} \langle p_x \rangle &= -i\hbar \int_{-\infty}^{\infty} \psi \frac{d\psi}{dx} \, dx = -i\hbar \frac{1}{2} \int_{-\infty}^{\infty} \frac{d}{dx} [\psi(x)]^2 dx \\ &= -\frac{1}{2} i\hbar [\psi^2(\infty) - \psi^2(-\infty)] = \underline{\underline{0}} \, . \end{aligned} \tag{3}$$

In the last line, we have used that $\psi(x)$ approaches zero for $x \to \pm\infty$.

In order to find $\langle p_x^2 \rangle$, we calculate

$$\frac{d\psi}{dx} = \left(\frac{2\beta}{\pi} \right)^{1/4} e^{-\beta(x-a)^2} [-2\beta(x-a)] = -2\beta(x-a)\psi \, , \tag{4}$$

and find that

$$\begin{aligned} \langle p_x^2 \rangle &= \int_{-\infty}^{\infty} \psi \hat{p}_x \hat{p}_x \psi \, dx = \int_{-\infty}^{\infty} |\hat{p}_x \psi|^2 \, dx = \hbar^2 \int_{-\infty}^{\infty} \left| \frac{d\psi}{dx} \right|^2 dx \\ &= 4\beta^2 \hbar^2 \int_{-\infty}^{\infty} (x-a)^2 |\psi|^2 dx = 4\beta^2 \hbar^2 (\Delta x)^2 = \beta \hbar^2, \end{aligned} \tag{5}$$

where we in the second equality have used the Hermitian property of $\hat{p}_x$ to move it to operate on the first ψ. Using this result, we find the uncertainty $\Delta p_x = \sqrt{\langle p_x^2 \rangle - \langle p_x \rangle^2} = \hbar\sqrt{\beta}$. We note that the product of the uncertainties for this type of Gaussian wave function is

$$\Delta x \Delta p_x = \frac{1}{2}\hbar, \tag{6}$$

which is the minimal value it can have according to Heisenberg's uncertainty relation ($\Delta x \Delta p_x \geq \frac{1}{2}\hbar$). This is agreement with the results from problem set 2. Moreover, by choosing a β large, we obtain a small uncertainty in the position, $\Delta x = 1/(2\sqrt{\beta})$. This, however, gives a large uncertainty in the momentum, $\Delta p_x = \hbar\sqrt{\beta}$.

d) The expectation value of the kinetic energy is

$$\langle E_k \rangle = \frac{1}{2m} \langle p_x^2 \rangle = \frac{\hbar^2 \beta}{2m} = \frac{\hbar^2}{8m(\Delta x)^2} \, . \tag{7}$$

If we let $\Delta x \to 0$, the average kinetic energy increases towards infinity.

Problem 2

a) Operating with $\hat{p}$ on $\psi(x)$, we get

$$-i\hbar\frac{d}{dx}\psi_n(x) = -i\frac{\hbar\pi n}{L}\sqrt{\frac{2}{L}}\cos\frac{\pi n x}{L} \neq \text{constant}\cdot\psi_n(x). \tag{8}$$

Hence, the energy eigenstates are not momentum eigenstates.

b) We get

$$\langle m|n\rangle = \langle m| \int dx \ \ |x\rangle\langle x|\,|n\rangle = \int dx \ \ \langle m|x\rangle\langle x|n\rangle = \int dx \ \psi_m^*(x)\psi_n(x). \tag{9}$$

Since the wavefunctions $\psi_n(x)$ nonzero only for $0 < x < L$, we can write this as

$$\langle m|n\rangle = \int_0^L dx \ \psi_m^*(x)\psi_n(x) = \delta_{mn}, \tag{10}$$

where we have used the given relation in the last equality.

c) Inserting a completeness relation for the position basis, and following similar steps as above, we directly get

$$\langle p|n\rangle = \int dx \ \ \langle p|x\rangle\langle x|n\rangle\,. \tag{11}$$

d) We insert

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar}, \tag{12}$$

and

$$\langle x|n\rangle = \sqrt{\frac{2}{L}}\sin\frac{\pi n x}{L} \tag{13}$$

into the expression for $\phi_n(p)$:

$$\begin{aligned}\phi_n(p) = \langle p|n\rangle &= \int dx \ \ \underbrace{\langle p|x\rangle}_{\langle x|\,p\rangle^*}\underbrace{\langle x|n\rangle}_{\psi_n(x)} = \int_0^L dx \ \sqrt{\frac{2}{L}\frac{1}{2\pi\hbar}}\sin\frac{\pi n x}{L}e^{-ipx/\hbar} \\ &= \frac{1}{\sqrt{\pi\hbar L}}\int_0^L dx \ \ \sin\frac{\pi n x}{L}e^{-ipx/\hbar}.\end{aligned} \tag{14}$$

To calculate the integral, we use $\sin x = \frac{e^{ix}-e^{-ix}}{2i}$:

$$\begin{aligned}
\phi_n(p) &= \frac{1}{2i\sqrt{\pi\hbar L}}\int_0^L dx\left[e^{ix\left(\frac{\pi n}{L}-\frac{p}{\hbar}\right)} - e^{-ix\left(\frac{\pi n}{L}+\frac{p}{\hbar}\right)}\right] \\
&= -\frac{1}{\sqrt{4\pi\hbar L}}\left[\frac{e^{ix\left(\frac{\pi n}{L}-\frac{p}{\hbar}\right)}}{\frac{\pi n}{L}-\frac{p}{\hbar}} + \frac{e^{-ix\left(\frac{\pi n}{L}+\frac{p}{\hbar}\right)}}{\frac{\pi n}{L}+\frac{p}{\hbar}}\right]\Bigg|_0^L \\
&= -\frac{1}{\sqrt{4\pi\hbar L}}\left[\frac{e^{i\left(\pi n-\frac{pL}{\hbar}\right)}-1}{\frac{\pi n}{L}-\frac{p}{\hbar}} + \frac{e^{-i\left(\pi n+\frac{pL}{\hbar}\right)}-1}{\frac{\pi n}{L}+\frac{p}{\hbar}}\right].
\end{aligned} \tag{15}$$

We now use $e^{\pm i\pi n} = (-1)^n$, and define the dimensionless quantity $P = pL/\hbar$ to simplify the notation, resulting in

$$\phi_n(P) = -\sqrt{\frac{L}{4\pi\hbar}}\left[\frac{(-1)^n e^{-iP}-1}{\pi n - P} + \frac{(-1)^n e^{-iP}-1}{\pi n + P}\right] = \sqrt{\frac{L\pi}{\hbar}}\frac{1-(-1)^n e^{-iP}}{(\pi n)^2 - P^2}n. \tag{16}$$

The probability density is then

$$|\phi_n(P)|^2 = \frac{2L\pi}{\hbar}n^2\,\frac{1-(-1)^n\cos P}{[(n\pi)^2-P^2]^2}. \tag{17}$$

Both the denominator and numerator is zero when $P = \pm n\pi$:

$$|\phi_n(\pm n\pi)|^2 = \frac{2L\pi}{\hbar}n^2\frac{1-(-1)^n(-1)^n}{[(n\pi)^2-(n\pi)^2]^2} = \frac{0}{0}. \tag{18}$$

Using L'Hôpital's rule, we get

$$\lim_{P\to\pm n\pi}|\phi_n(P)|^2 = \lim_{P\to\pm n\pi}\frac{2L\pi}{\hbar}n^2\frac{(-1)^n\sin P}{-4[(n\pi)^2-P^2]P} = \lim_{P\to\pm n\pi} -\frac{L\pi}{2\hbar}n^2\frac{(-1)^n\cos P}{(n\pi)^2-3P^2} = \frac{L}{4\pi\hbar}. \tag{19}$$

A plot of the probability density for $n = 1, 2, 3$ is show in fig. 1, showing that the energy eigenstates correspond to a superposition of *many* momentum states, with the peaks moving to increasing $|p|$ for higher energy states.

Problem 3

a) By adding and subtracting the ladder operators, we get

$$a + a^\dagger = \sqrt{\frac{2m\omega}{\hbar}}\hat{x} \qquad \Rightarrow \qquad \hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(a^\dagger + a), \tag{20}$$

$$a - a^\dagger = i\sqrt{\frac{2}{\hbar m\omega}}\hat{p} \qquad \Rightarrow \qquad \hat{p} = i\sqrt{\frac{\hbar m\omega}{2}}(a^\dagger - a). \tag{21}$$

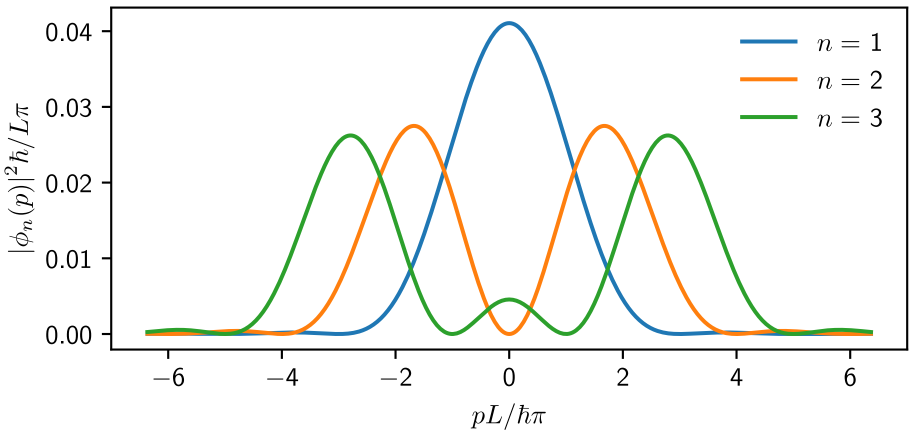

Figure 1: Plot of $|\phi_n(p)|^2$ as a function of p for $n = 1, 2, 3$.

The expectation values $\langle x \rangle$ and $\langle p \rangle$ are, therefore, proportional to

$$\langle n| a^\dagger \pm a |n\rangle = \sqrt{n+1} \langle n|n+1\rangle \pm \sqrt{n} \langle n|n-1\rangle = 0, \tag{22}$$

where the last equality follows from the fact that the states $|n\rangle$ are orthonormal, $\langle n|m\rangle = \delta_{nm}$. Hence, the expectation values of x and p are zero

b) The dual vector of

$$|\psi\rangle = A |n\rangle + B |m\rangle, \tag{23}$$

is

$$\langle \psi| = \langle n| A^* + \langle m| B^*. \tag{24}$$

If $|\psi\rangle$ is normalized, we must have

$$\begin{aligned} \langle \psi|\psi\rangle &= 1 \\ &= (\langle n| A^* + \langle m| B^*)(A |n\rangle + B |m\rangle) = |A|^2 + |B|^2, \end{aligned} \tag{25}$$

where we have used the orthonormality of the states. Hence, we must have

$$|A|^2 + |B|^2 = 1. \tag{26}$$

c) Using the expression for $\hat{x}$ in terms of the ladder operators found above, we get

$$\begin{aligned}
\langle x\rangle &= \langle\psi| x |\psi\rangle = \sqrt{\frac{\hbar}{2m\omega}}(\langle n| A^* + \langle m| B^*)(a^\dagger + a)(A|n\rangle + B|m\rangle) \\
&= \sqrt{\frac{\hbar}{2m\omega}}\,(\langle n| A^* + \langle m| B^*) \\
&\quad \times \left(A\sqrt{n+1}\,|n+1\rangle + A\sqrt{n}\,|n-1\rangle + B\sqrt{m+1}\,|m+1\rangle + B\sqrt{m}\,|m-1\rangle\right) \\
&= \sqrt{\frac{\hbar}{2m\omega}}\Big[A^*B\left(\sqrt{m+1}\,\langle n|m+1\rangle + \sqrt{m}\,\langle n|m-1\rangle\right) \\
&\quad + B^*A\left(\sqrt{n+1}\,\langle m|n+1\rangle + \sqrt{n}\,\langle m|n-1\rangle\right)\Big].
\end{aligned} \tag{27}$$

Since the states are orthonormal, we must have $m = n \pm 1$ in order for $\langle x\rangle \neq 0$. In that case, we get

$$\begin{aligned}
\langle x\rangle_\pm &= \sqrt{\frac{\hbar}{2m\omega}}\Big[A^*B\left(\sqrt{n\pm 1+1}\,\langle n|n\pm 1+1\rangle + \sqrt{n\pm 1}\,\langle n|n\pm 1-1\rangle\right) \\
&\quad + B^*A\left(\sqrt{n+1}\,\langle n\pm 1|n+1\rangle + \sqrt{n}\,\langle n\pm 1|n-1\rangle\right)\Big] \\
&= \begin{cases} \sqrt{\frac{2\hbar}{m\omega}}\sqrt{n+1}\;\Re\mathrm{e}(A^*B), & m = n+1, \\ \sqrt{\frac{2\hbar}{m\omega}}\sqrt{n}\;\Re\mathrm{e}(A^*B), & m = n-1. \end{cases}
\end{aligned} \tag{28}$$