

1. **McIntyre 9.9** (expectation values by integration and by operator method).

i) Write the wave function using the constant  $\beta^2 = m\omega/\hbar$ :

$$\varphi_0(x) = \left( \frac{m\omega}{\pi\hbar} \right)^{1/4} e^{-m\omega x^2/2\hbar} = \left( \frac{\beta^2}{\pi} \right)^{1/4} e^{-\beta^2 x^2/2}$$

The expectation value of position is

$$\langle x \rangle = \int_{-\infty}^{\infty} \varphi_0^*(x) x \varphi_0(x) dx = \int_{-\infty}^{\infty} x |\varphi_0(x)|^2 dx = 0$$

by symmetry since  $|\varphi_0(x)|^2$  is even. For momentum:

$$\begin{aligned} \langle p \rangle &= \int_{-\infty}^{\infty} \varphi_0^*(x) \frac{\hbar}{i} \frac{d}{dx} \varphi_0(x) dx = \int_{-\infty}^{\infty} \left( \frac{\beta^2}{\pi} \right)^{1/4} e^{-\beta^2 x^2/2} \frac{\hbar}{i} \frac{d}{dx} \left( \frac{\beta^2}{\pi} \right)^{1/4} e^{-\beta^2 x^2/2} dx \\ &= \left( \frac{\beta^2}{\pi} \right)^{1/2} \frac{\hbar}{i} \int_{-\infty}^{\infty} e^{-\beta^2 x^2/2} (-\beta^2 x) e^{-\beta^2 x^2/2} dx = \left( \frac{\beta^2}{\pi} \right)^{1/2} \frac{\hbar}{i} (-\beta^2) \int_{-\infty}^{\infty} x e^{-\beta^2 x^2} dx \\ &= 0 \end{aligned}$$

For the squares:

$$\begin{aligned} \langle x^2 \rangle &= \int_{-\infty}^{\infty} \varphi_0^*(x) x^2 \varphi_0(x) dx = \int_{-\infty}^{\infty} \left( \frac{\alpha}{\pi} \right)^{1/4} e^{-\alpha x^2/2} x^2 \left( \frac{\alpha}{\pi} \right)^{1/4} e^{-\alpha x^2/2} dx \\ &= \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} x^2 e^{-\alpha x^2} dx = \sqrt{\frac{\alpha}{\pi}} \frac{1}{2\alpha} \sqrt{\frac{\pi}{\alpha}} = \frac{1}{2\alpha} = \frac{\hbar}{2m\omega} \\ \langle p^2 \rangle &= \int_{-\infty}^{\infty} \varphi_0^*(x) \left( \frac{\hbar}{i} \frac{d}{dx} \right)^2 \varphi_0(x) dx = -\hbar^2 \sqrt{\frac{\beta^2}{\pi}} \int_{-\infty}^{\infty} e^{-\beta^2 x^2/2} \left( \frac{d}{dx} \right)^2 e^{-\beta^2 x^2/2} dx \\ &= -\hbar^2 \sqrt{\frac{\beta^2}{\pi}} \int_{-\infty}^{\infty} (\beta^4 x^2 - \beta^2) e^{-\beta^2 x^2} dx = -\hbar^2 \sqrt{\frac{\beta^2}{\pi}} \left[ \beta^4 \frac{1}{2\beta^2} \sqrt{\frac{\pi}{\beta^2}} - \beta^2 \sqrt{\frac{\pi}{\beta^2}} \right] = \frac{\beta^2 \hbar^2}{2} \\ &= \frac{m\omega \hbar}{2} \end{aligned}$$

ii) Now do the same for all states but using the operators  $a$  and  $a^\dagger$ .

$$a = \frac{1}{\sqrt{2\hbar m\omega}}(-ip + m\omega x)$$

$$a^\dagger = \frac{1}{\sqrt{2\hbar m\omega}}(ip + m\omega x)$$

$$x = \sqrt{\frac{\hbar}{2m\omega}}(a^\dagger + a)$$

$$p = i\sqrt{\frac{\hbar m\omega}{2}}(a^\dagger - a)$$

$$\begin{aligned}\langle x \rangle &= \langle n | x | n \rangle = \sqrt{\frac{\hbar}{2m\omega}} \langle n | a^\dagger + a | n \rangle \\ &= \sqrt{\frac{\hbar}{2m\omega}} [\langle n | a^\dagger | n \rangle + \langle n | a | n \rangle] = \sqrt{\frac{\hbar}{2m\omega}} [\langle n | \sqrt{n+1} | n+1 \rangle + \langle n | \sqrt{n} | n-1 \rangle] \\ &= \sqrt{\frac{\hbar}{2m\omega}} [\sqrt{n+1} \langle n | n+1 \rangle + \sqrt{n} \langle n | n-1 \rangle] = 0 \text{ since } \langle n | m \rangle = \delta_{nm}\end{aligned}$$

$$\begin{aligned}\langle p \rangle &= \langle n | p | n \rangle = \sqrt{\frac{\hbar}{2m\omega}} \langle n | a^\dagger - a | n \rangle \\ &= \sqrt{\frac{\hbar}{2m\omega}} [\langle n | a^\dagger | n \rangle - \langle n | a | n \rangle] = \sqrt{\frac{\hbar}{2m\omega}} [\langle n | \sqrt{n+1} | n+1 \rangle - \langle n | \sqrt{n} | n-1 \rangle] \\ &= \sqrt{\frac{\hbar}{2m\omega}} [\sqrt{n+1} \langle n | n+1 \rangle - \sqrt{n} \langle n | n-1 \rangle] = 0 \text{ since } \langle n | m \rangle = \delta_{nm}\end{aligned}$$

Note also that  $\langle n | a^2 | n \rangle = 0$  and  $\langle n | (a^\dagger)^2 | n \rangle = 0$  in a similar manner, so that

$$\begin{aligned}\langle x^2 \rangle &= \langle n | x^2 | n \rangle = \frac{\hbar}{2m\omega} \langle n | (a^\dagger + a)^2 | n \rangle = \frac{\hbar}{2m\omega} \langle n | (a^\dagger)^2 + a^\dagger a + a a^\dagger + a^2 | n \rangle \\ &= \frac{\hbar}{2m\omega} \langle n | a^\dagger a + a a^\dagger | n \rangle = \frac{\hbar}{2m\omega} \langle n | \sqrt{n} \sqrt{n} + \sqrt{n+1} \sqrt{n+1} | n \rangle \\ &= \frac{\hbar}{2m\omega} (2n+1) = \frac{\hbar}{m\omega} \left(n + \frac{1}{2}\right)\end{aligned}$$

$$\begin{aligned}\langle p^2 \rangle &= \langle n | p^2 | n \rangle = -\frac{\hbar m\omega}{2} \langle n | (a^\dagger - a)^2 | n \rangle = -\frac{\hbar m\omega}{2} \langle n | (a^\dagger)^2 - a^\dagger a - a a^\dagger + a^2 | n \rangle \\ &= \frac{\hbar m\omega}{2} \langle n | a^\dagger a + a a^\dagger | n \rangle = \frac{\hbar}{2m\omega} \langle n | \sqrt{n} \sqrt{n} + \sqrt{n+1} \sqrt{n+1} | n \rangle \\ &= \frac{\hbar m\omega}{2} (2n+1) = \hbar m\omega \left(n + \frac{1}{2}\right)\end{aligned}$$

All of these agree with part (i)

iii) The uncertainty principle is  $\Delta x \Delta p \geq \hbar/2$  where

$$\Delta x = \sqrt{\langle (x - \langle x \rangle)^2 \rangle} = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sqrt{\langle x^2 \rangle} \quad \text{since } \langle x \rangle = 0$$

$$\Delta p = \sqrt{\langle (p - \langle p \rangle)^2 \rangle} = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \sqrt{\langle p^2 \rangle} \quad \text{since } \langle p \rangle = 0$$

$$\Delta x = \sqrt{\frac{\hbar}{m\omega}(n + \frac{1}{2})}$$

$$\Delta p = \sqrt{\hbar m\omega(n + \frac{1}{2})}$$

$$\Delta x \Delta p = \sqrt{\frac{\hbar}{m\omega}(n + \frac{1}{2})} \sqrt{\hbar m\omega(n + \frac{1}{2})} = (n + \frac{1}{2})\hbar \geq \frac{\hbar}{2}$$

The uncertainty relation is obeyed for all states and the minimum uncertainty is realized in the ground state (Gaussian wave function).

## 2. McIntyre 9.14 (expectation values)

a) To solve this problem, write the state in terms of energy eigenstates. Rather than calculating the coefficients using spatial overlap integrals, try to write the state in a way that makes it obvious which energy states are included. First write out the harmonic oscillator functions to see how they relate to this state. To simplify notation, use the standard variable change  $\xi = \sqrt{m\omega/\hbar} x = \beta x$ :

$$\varphi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-m\omega x^2/2\hbar} = \left(\frac{\beta^2}{\pi}\right)^{\frac{1}{4}} e^{-\beta^2 x^2/2} = \left(\frac{\beta^2}{\pi}\right)^{\frac{1}{4}} e^{-\xi^2/2}$$

$$\varphi_1(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \sqrt{\frac{m\omega}{\hbar}} \frac{1}{\sqrt{2}} 2x e^{-m\omega x^2/2\hbar} = \left(\frac{\beta^2}{\pi}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2}} 2\beta x e^{-\beta^2 x^2/2} = \left(\frac{\beta^2}{\pi}\right)^{\frac{1}{4}} \sqrt{2} \xi e^{-\xi^2/2}$$

$$\varphi_2(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \frac{1}{\sqrt{8}} [4 \frac{m\omega}{\hbar} x^2 - 2] e^{-m\omega x^2/2\hbar} = \left(\frac{\beta^2}{\pi}\right)^{\frac{1}{4}} \frac{1}{\sqrt{8}} [4\beta^2 x^2 - 2] e^{-\beta^2 x^2/2} = \left(\frac{\beta^2}{\pi}\right)^{\frac{1}{4}} \frac{1}{\sqrt{8}} [4\xi^2 - 2] e^{-\xi^2/2}$$

$$\Rightarrow e^{-\xi^2/2} = \varphi_0(x) \left(\frac{\pi}{\beta^2}\right)^{\frac{1}{4}}; \quad \xi e^{-\xi^2/2} = \frac{1}{\sqrt{2}} \varphi_1(x) \left(\frac{\pi}{\beta^2}\right)^{\frac{1}{4}}; \quad [2\xi^2 - 1] e^{-\xi^2/2} = \sqrt{2} \varphi_2(x) \left(\frac{\pi}{\beta^2}\right)^{\frac{1}{4}}$$

The initial wave function is thus

$$\begin{aligned} \psi(x, 0) &= A \left( 1 - 3\sqrt{\frac{m\omega}{\hbar}} x + 2\frac{m\omega}{\hbar} x^2 \right) e^{-m\omega x^2/2\hbar} = A \left( 1 - 3\beta x + 2\beta^2 x^2 \right) e^{-\beta^2 x^2/2} \\ &= A \left( 1 - 3\xi + 2\xi^2 \right) e^{-\xi^2/2} = A \left( 2(1) - 3(\xi) + 1(2\xi^2 - 1) \right) e^{-\xi^2/2} \\ &= A \left( \frac{\pi}{\beta^2} \right)^{\frac{1}{4}} \left( 2\varphi_0(x) - \frac{3}{\sqrt{2}} \varphi_1(x) + \sqrt{2} \varphi_2(x) \right) \end{aligned}$$

Switching to bra-ket notation, we have

$$|\psi(0)\rangle = C \left( 2|0\rangle - \frac{3}{\sqrt{2}}|1\rangle + \sqrt{2}|2\rangle \right)$$

where  $C$  is the normalization constant. Normalize to find  $C$

$$\begin{aligned} 1 &= |\langle \psi(0) | \psi(0) \rangle| = |C|^2 \left( 2\langle 0 | - \frac{3}{\sqrt{2}}\langle 1 | + \sqrt{2}\langle 2 | \right) \left( 2|0\rangle - \frac{3}{\sqrt{2}}|1\rangle + \sqrt{2}|2\rangle \right) \\ &= |C|^2 (4 + \frac{9}{2} + 2) = \frac{21}{2} |C|^2 \quad \Rightarrow C = \frac{\sqrt{2}}{\sqrt{21}} \end{aligned}$$

Now find the expectation value of the energy:

$$\begin{aligned} \langle E \rangle &= \sum_n E_n \delta_{E_n} = \sum_n (n + \frac{1}{2}) \hbar \omega \delta_{E_n} \\ \delta_{E_n} &= |\langle n | \psi(0) \rangle|^2 = \left| \langle n | \frac{\sqrt{2}}{\sqrt{21}} (2|0\rangle - \frac{3}{\sqrt{2}}|1\rangle + \sqrt{2}|2\rangle) \right|^2 = \frac{2}{21} \left| 2\langle n | 0 \rangle - \frac{3}{\sqrt{2}}\langle n | 1 \rangle + \sqrt{2}\langle n | 2 \rangle \right|^2 \\ &= \frac{2}{21} (4\delta_{n0} + \frac{9}{2}\delta_{n1} + 2\delta_{n2}) \\ \langle E \rangle &= \sum_n (n + \frac{1}{2}) \hbar \omega \frac{2}{21} (4\delta_{n0} + \frac{9}{2}\delta_{n1} + 2\delta_{n2}) = \frac{2}{21} \hbar \omega [4 \frac{1}{2} + \frac{9}{2} \frac{3}{2} + 2 \frac{5}{2}] = \frac{2}{21} \hbar \omega [2 + \frac{27}{4} + 5] \\ &= \frac{55}{42} \hbar \omega \approx 1.31 \hbar \omega \end{aligned}$$

### 3. Commutator algebra

(a) Show that the following are true. You don't need to reflect on the physics,

$$[\hat{A}, (\hat{B} + \hat{C})] = \hat{A}(\hat{B} + \hat{C}) - (\hat{B} + \hat{C})\hat{A} = \hat{A}\hat{B} + \hat{A}\hat{C} - (\hat{B}\hat{A} + \hat{C}\hat{A}) = [\hat{A}, \hat{B}] + [\hat{A}, \hat{C}]$$

(the distributive law holds)

$$\begin{aligned} [\hat{A}, \hat{B}\hat{C}] &= \hat{A}\hat{B}\hat{C} - \hat{B}\hat{C}\hat{A} = \hat{A}\hat{B}\hat{C} - \hat{B}\hat{A}\hat{C} - \hat{B}\hat{C}\hat{A} + \hat{B}\hat{A}\hat{C} \\ &= \{\hat{A}\hat{B} - \hat{B}\hat{A}\} \hat{C} + \hat{B} \{-\hat{C}\hat{A} + \hat{A}\hat{C}\} \\ &= [\hat{A}, \hat{B}] \hat{C} + \hat{B} [\hat{A}, \hat{C}] \end{aligned}$$

(b) Show that  $[\hat{x}, \hat{p}] = i\hbar$ . Hint: operate on a general wave function and use the position representation of the operators.

The right hand side SHOULD be an operator, because the left hand side is, but it looks like a number. We interpret the number as being multiplied by the identity operator, which can take many forms, depending on the situation. In matrix mechanics, for example, it's a square matrix with the number 1 as every diagonal element.

To prove the identity, operate with the commutator on some arbitrary function of  $x$ ,

$$\begin{aligned} [\hat{x}, \hat{p}] \phi &= \left[ x, -i\hbar \frac{d}{dx} \right] \phi(x) = -i\hbar \left[ x, i\hbar \frac{d}{dx} \right] \phi(x) = -i\hbar \left\{ x \frac{d}{dx} \phi(x) - \frac{d}{dx} (x\phi(x)) \right\} \\ &= -i\hbar \left\{ x \frac{d\phi(x)}{dx} - \frac{dx}{dx} \phi(x) - x \frac{d\phi(x)}{dx} \right\} = -i\hbar \left\{ x \frac{d\phi(x)}{dx} - \phi(x) - x \frac{d\phi(x)}{dx} \right\} \\ &= i\hbar \phi(x) \end{aligned}$$

Be very careful about the chain rule and what is operating on what. Now if

$$[x, p] \phi(x) = i\hbar \phi(x) \text{ then } [x, p] = i\hbar \mathbf{1} \text{ with the bold 1 the identity operator.}$$

HO	Ket Representation	Wave Function Representation	Matrix Representation
Hamiltonian	$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$ $= (a^\dagger a + \frac{1}{2})\hbar\omega_0$	$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2x^2$	$H = \begin{pmatrix} \frac{1}{2}\hbar\omega & 0 & 0 & \dots \\ 0 & \frac{3}{2}\hbar\omega & 0 & \dots \\ 0 & 0 & \frac{5}{2}\hbar\omega & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$
Eigenvalues of Hamiltonian	$E_n = \left(n + \frac{1}{2}\right)\hbar\omega$ $n = 0, 1, 2, 3, \dots$	$E_n = \left(n + \frac{1}{2}\right)\hbar\omega$ $n = 0, 1, 2, 3, \dots$	$E_n = \left(n + \frac{1}{2}\right)\hbar\omega$ $n = 0, 1, 2, 3, \dots$
Normalized eigenstates of Hamiltonian	$ n\rangle$	$ \varphi_n(x)\rangle$ $\varphi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\xi^2/2}$ $\xi \equiv \sqrt{\frac{m\omega}{\hbar}} x$	$ 0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix}, \quad  1\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad \dots$
Matrix element/matrix of position operator	$X_{nm} = \langle n   X   m \rangle = \sqrt{\frac{\hbar}{2m\omega}} (\sqrt{m}\delta_{n,m-1} + \sqrt{m+1}\delta_{n,m+1})$	$X_{nm} = \text{(integral)}$ $= \int_{-\infty}^{+\infty} \varphi_n(x) x \varphi_m(x) dx \quad (\text{note that harmonic oscillator wavefunctions are real})$	$X := \text{(matrix)} = \sqrt{\frac{\hbar}{2m\omega}} \begin{pmatrix} 0 & \sqrt{1} & 0 & \dots \\ \sqrt{1} & 0 & \sqrt{2} & \dots \\ 0 & \sqrt{2} & 0 & \vdots \end{pmatrix}$ <p>(see Eq. 9.96 in McIntyre)</p>
Matrix element/matrix of momentum operator	$P_{nm} = \langle n   P   m \rangle = -i\sqrt{\frac{\hbar m \omega}{2}} (\sqrt{m}\delta_{n,m-1} - \sqrt{m+1}\delta_{n,m+1})$	$P_{nm} = \text{(integral)}$ $= \int_{-\infty}^{+\infty} \varphi_n(x) (-i\hbar) \frac{d\varphi_m(x)}{dx} dx$	$P := \text{(matrix)} = \sqrt{\frac{\hbar m \omega}{2}} \begin{pmatrix} 0 & -i\sqrt{1} & 0 & \dots \\ i\sqrt{1} & 0 & -i\sqrt{2} & \dots \\ 0 & i\sqrt{2} & 0 & \vdots \end{pmatrix}$ <p>(see Eq. 9.96 in McIntyre)</p>