**PHY V2500: QUANTUM MECHANICS I**

**Problem Set 3**

**Due October 7, 2025**

---

## Problem 1

In the discussion of the harmonic oscillator in class, I introduced the operators

$$a = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + \frac{i}{\sqrt{2m\hbar\omega}}\hat{p}, \qquad a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} - \frac{i}{\sqrt{2m\hbar\omega}}\hat{p}$$

I also showed that the eigenstates of the Hamiltonian are given by

$$|n\rangle = \frac{1}{\sqrt{n!}}(a^\dagger)^n |0\rangle$$

a) Writing $\hat{x}$ and $\hat{p}$ in terms of $a$ and $a^\dagger$, obtain the matrix elements of the momentum operator defined by

$$P_{mn} = \langle m| \hat{p} |n\rangle$$

(*Do not try to write an infinite-dimensional matrix; use the Kronecker delta to make the notation compact.*)

b) We define the operators

$$R_+ = \tfrac{1}{2}(a^\dagger)^2, \qquad R_- = \tfrac{1}{2}(a)^2, \qquad R_3 = a^\dagger a + \tfrac{1}{2}$$

Work out the commutation rules $[R_+, R_-]$, $[R_3, R_\pm]$.

c) Calculate the matrix elements $\langle n| R_\pm |m\rangle$.

## Solution

a) From the definition of $a$ and $a^\dagger$, we find

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(a^\dagger + a), \qquad \hat{p} = i\sqrt{\frac{m\hbar\omega}{2}}(a^\dagger - a)$$

The action of the step-up and step-down operators is given by

$$a|n\rangle = \sqrt{n}\,|n-1\rangle\,,\ a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle$$

The matrix elements of the momentum operator are thus

$$\begin{aligned} P_{mn} &= \langle m|\hat{p}|n\rangle = i\sqrt{\frac{m\hbar\omega}{2}}(\langle m|a^\dagger|n\rangle - \langle m|a|n\rangle) \\ &= i\sqrt{\frac{m\hbar\omega}{2}}(\sqrt{n+1}\,\langle m|n+1\rangle - \sqrt{n}\,\langle m|n-1\rangle) \\ &= i\sqrt{\frac{m\hbar\omega}{2}}(\sqrt{n+1}\delta_{m,n+1} - \sqrt{n}\delta_{m,n-1}) \end{aligned}$$

b) The basic commutation rule we need is

$$aa^\dagger - a^\dagger a = [a, a^\dagger] = 1$$

We can also use the rules (worked out in class)

$$[A, BC] = [A, B]\, C + B\, [A, C], \qquad [AB, C] = [A, C]\, B + A\, [B, C]$$

Using these

$$\begin{aligned}
[R_+, R_-] &= \frac{1}{4}[a^{\dagger 2}, a^2] = \frac{1}{4}\Big(a^\dagger[a^\dagger, a^2] + [a^\dagger, a^2]a^\dagger\Big) \\
&= \frac{1}{4}\Big(a^\dagger\big([a^\dagger, a]a + a[a^\dagger, a]\big) + \big([a^\dagger, a]a + a[a^\dagger, a]\big)a^\dagger\Big) \\
&= -\frac{1}{4}\Big(2a^\dagger a + 2aa^\dagger\Big) = -\frac{1}{4}\Big(4a^\dagger a + 2\Big) \\
&= -R_3
\end{aligned}$$

Similarly

$$\begin{aligned}
[R_3, R_+] &= \frac{1}{2}[a^\dagger a + \tfrac{1}{2}, a^{\dagger 2}] = \frac{1}{2}a^\dagger [a, a^{\dagger 2}] = \frac{1}{2}a^\dagger\Big(a^\dagger[a, a^\dagger] + [a, a^\dagger]a^\dagger\Big) \\
&= (a^\dagger)^2 = 2\, R_+
\end{aligned}$$

Also notice that $(R_+)^\dagger = R_-$. So taking the hermitian conjugate of the equation given above we get

$$[R_3, R_-] = -2\, R_-$$

c) For this part we can use the simplification of $a\,|n\rangle$ and $a^\dagger\,|n\rangle$ given above. Thus

$$\begin{aligned}
\langle n|\, R_+\, |m\rangle &= \frac{1}{2}\,\langle n|\, a^\dagger a^\dagger\, |m\rangle = \tfrac{1}{2}\sqrt{(m+1)(m+2)}\ \langle n|m+2\rangle \\
&= \tfrac{1}{2}\sqrt{(m+1)(m+2)}\,\delta_{n,m+2} \\
\langle n|\, R_-\, |m\rangle &= \frac{1}{2}\,\langle n|\, aa\, |m\rangle = \tfrac{1}{2}\sqrt{m(m-1)}\ \langle n|m-2\rangle \\
&= \tfrac{1}{2}\sqrt{m(m-1)}\,\delta_{n,m-2}
\end{aligned}$$

**Problem 2**

In this problem you will check orthonormality of two of the energy eigenstates for the oscillator using the explicit formulae for the wave functions. Consider the first and second excited states of the oscillator given by the wave functions

$$\begin{aligned}
\psi_1(x) = \langle x|1\rangle &= \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2}} H_1(\xi)\, e^{-\frac{1}{2}\xi^2} \\
\psi_2(x) = \langle x|2\rangle &= \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \frac{1}{\sqrt{8}} H_2(\xi)\, e^{-\frac{1}{2}\xi^2} \\
H_1(\xi) = 2\xi, &\qquad\qquad H_2(\xi) = 4\xi^2 - 2
\end{aligned}$$

where $\xi = \sqrt{m\omega/\hbar}\, x$.

a) Calculate $\langle 1|1\rangle$, $\langle 2|2\rangle$, $\langle 1|2\rangle$ using the definition of the inner product

$$\langle n|m\rangle = \int_{-\infty}^{\infty} dx\, \psi_n^*\, \psi_m$$

(*You must show how you worked out the integrals.*)

**Solution**

With the given wave functions, we have

$$\begin{aligned}\langle 1|1\rangle &= \frac{1}{\sqrt{\pi}}\frac{1}{2}\int_{-\infty}^{\infty} d\xi H_1^2\, e^{-\xi^2}\\ \langle 2|2\rangle &= \frac{1}{\sqrt{\pi}}\frac{1}{8}\int_{-\infty}^{\infty} d\xi H_2^2\, e^{-\xi^2}\\ \langle 1|2\rangle &= \frac{1}{\sqrt{\pi}}\frac{1}{4}\int_{-\infty}^{\infty} d\xi H_1 H_2\, e^{-\xi^2}\end{aligned}$$

We can evaluate the needed integrals as follows.

$$\int_{-\infty}^{\infty} d\xi\, \xi^n\, e^{-\xi^2} = 0$$

if $n$ is an odd integer. From the given $H_1$ and $H_2$, we see that $H_1 H_2$ is odd, so we immediately have $\langle 1|2\rangle = 0$. Now consider the integral

$$\int_{-\infty}^{\infty} d\xi\, e^{-a\xi^2} = \sqrt{\pi}\, a^{-\frac{1}{2}}$$

Differentiating this with respect to $a$ and setting it to 1, we find

$$\begin{aligned}I_0 = \int_{-\infty}^{\infty} d\xi\, e^{-\xi^2} &= \sqrt{\pi}\\ I_2 = \int_{-\infty}^{\infty} d\xi\, \xi^2\, e^{-\xi^2} &= -\frac{\partial}{\partial a}\sqrt{\pi}\, a^{-\frac{1}{2}}\Big|_{a=1} = \frac{1}{2}\sqrt{\pi}\\ I_4 = \int_{-\infty}^{\infty} d\xi\, \xi^4\, e^{-\xi^2} &= \frac{\partial^2}{\partial a^2}\sqrt{\pi}\, a^{-\frac{1}{2}}\Big|_{a=1} = \frac{3}{4}\sqrt{\pi}\end{aligned}$$

Using these

$$\begin{aligned}\langle 1|1\rangle &= \frac{1}{2\sqrt{\pi}}\, 4\, I_2 = 1\\ \langle 2|2\rangle &= \frac{1}{8\sqrt{\pi}}\int d\xi\, (16\xi^4 - 16\xi^2 + 4)e^{-\xi^2}\\ &= \frac{1}{8\sqrt{\pi}}\left(\frac{16\times 3}{4} - 16\times\frac{1}{2} + 4\right)\sqrt{\pi} = 1\end{aligned}$$

**Problem 3**

Consider the harmonic oscillator with the eigenfunctions $\psi_n$ of the Hamiltonian as given in class. We take a state at time $t = 0$ given by

$$\psi = A(\psi_0 + \psi_1)$$

a) Find the normalization factor $A$.
b) Consider the wave function at time $t$ and calculate $\langle x \rangle$ and $\langle p \rangle$ at time $t$ using these wave functions. (Your answers will have some time dependence.)
c) Show that for *every odd value of* $n$, the eigenfunctions $\psi_n(x)$ of the Hamiltonian for the oscillator vanish at $x = 0$.

**Solution**
a) The wave functions $\psi_0$ and $\psi_1$ are orthonormal. Thus

$$\int dx\, \psi^* \psi = |A|^2 \left[\langle 0|0\rangle + \langle 0|1\rangle + \langle 1|0\rangle + \langle 1|1\rangle\right] = |A|^2\, 2 \equiv 1$$

This identifies $A = (1/\sqrt{2})$, up to a phase.
b) The wave function at time $t$ is given by

$$\psi(t) = \frac{1}{\sqrt{2}} \left[ e^{-i\omega t/2} \langle x|0\rangle + e^{-i3\omega t/2} \langle x|1\rangle \right]$$

From the expressions for $x$ and $p$ given in Problem 1,

$$\langle 0|\, x\, |0\rangle = \langle 1|\, x\, |1\rangle = 0, \qquad \langle 0|\, x\, |1\rangle = \sqrt{\frac{\hbar}{2m\omega}},\ \ \langle 1|\, x\, |0\rangle = \sqrt{\frac{\hbar}{2m\omega}}$$
$$\langle 0|\, p\, |0\rangle = \langle 1|\, p\, |1\rangle = 0, \qquad \langle 0|\, p\, |1\rangle = -i\sqrt{\frac{m\hbar\omega}{2}},\ \ \langle 1|\, p\, |0\rangle = i\sqrt{\frac{m\hbar\omega}{2}}$$

Thus

$$\begin{aligned}
\langle \psi, t|\, x\, |\psi, t\rangle &= \frac{1}{2}\left[\langle 0|\, x\, |0\rangle + \langle 1|\, x\, |1\rangle + e^{-i\omega t} \langle 0|\, x\, |1\rangle + e^{i\omega t} \langle 1|\, x\, |0\rangle\right] \\
&= \sqrt{\frac{\hbar}{2m\omega}} \cos\omega t \\
\langle \psi, t|\, p\, |\psi, t\rangle &= \frac{1}{2}\left[\langle 0|\, p\, |0\rangle + \langle 1|\, p\, |1\rangle + e^{-i\omega t} \langle 0|\, p\, |1\rangle + e^{i\omega t} \langle 1|\, p\, |0\rangle\right] \\
&= -\sqrt{\frac{m\hbar\omega}{2}} \sin\omega t
\end{aligned}$$

Notice that $\langle p \rangle = m\frac{d}{dt}\langle x \rangle$.
c) The wave functions for the energy eigenstates of the oscillator were obtained in class as

$$\psi_n(x) = \langle x|n\rangle = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n\, n!}} H_n(\xi)\, e^{-\frac{1}{2}\xi^2}$$

where the Hermite polynomials $H_n(\xi)$ are given by

$$\left(\xi - \frac{\partial}{\partial\xi}\right)^n e^{-\frac{1}{2}\xi^2} = H_n(\xi)\, e^{-\frac{1}{2}\xi^2}$$

$\xi$ is proportional to $x$ and hence the combination $\xi - \frac{\partial}{\partial \xi}$ changes sign under $x \to -x$. Therefore the odd Hermite polynomials are odd functions of $x$, i.e., $H_n(-x) = -H_n(x)$. Thus $H_n(0) = 0$ for odd values of $n$, showing that the wave functions for odd $n$ will vanish at $x = 0$.

**Problem 4**

Consider a particle which can move in one dimension, but on the *half-line* $0 \leq x \leq \infty$. Write down the condition for hermiticity of the momentum operator. What is the boundary condition on the wave functions at $x = 0$ to ensure that the momentum operator has the right hermiticity property?

**Solution**

Since the particle is on the interval $0 \leq x \leq \infty$, the condition for hermiticity of the momentum operator $p = -i\hbar(\partial/\partial x)$ is

$$\int_0^\infty dx\, \psi_1^* \left(-i\hbar \frac{\partial \psi_2}{\partial x}\right) = \int_0^\infty dx\, \left(-i\hbar \frac{\partial \psi_1}{\partial x}\right)^* \psi_2$$

The right hand side of this equation, using integration by parts, is

$$\begin{aligned}\int_0^\infty dx\, \left(-i\hbar \frac{\partial \psi_1}{\partial x}\right)^* \psi_2 &= \int_0^\infty dx\, i\hbar \frac{\partial \psi_1}{\partial x}^* \psi_2 = -i\hbar \int_0^\infty dx\, \psi_1^* \frac{\partial \psi_2}{\partial x} + i\hbar\, \psi_1^* \psi_2 \Big]_0^\infty \\ &= \int_0^\infty dx\, \psi_1^* \left(-i\hbar \frac{\partial \psi_2}{\partial x}\right) + i\hbar\, \psi_1^* \psi_2 \Big]_0^\infty\end{aligned}$$

We see that the hermiticity condition is satisfied if

$$\psi_1^* \psi_2 \Big]_0^\infty = \psi_1^*(\infty)\psi_2(\infty) - \psi_1^*(0)\, \psi_2(0) = 0$$

For normalizable wave functions for which we have $\psi(\infty) = 0$, this reduces to $\psi(0) = 0$ for all wave functions, since the above equation should hold for any choice of $\psi_1$, $\psi_2$.