Peeter Joot
peeterjoot@protonmail.com

Expectations for SHO Hamiltonian, and virial theorem.

Exercise 1.1 **Expectations for SHO Hamiltonian, and virial theorem.** ([1] *pr. 2.3*)

1. For a 1D SHO, compute $\left\langle m \right| x \left| n \right\rangle$, $\left\langle m \right| x^2 \left| n \right\rangle$, $\left\langle m \right| p \left| n \right\rangle$, $\left\langle m \right| p^2 \left| n \right\rangle$ and $\left\langle m \right| \left\{ x, p \right\} \left| n \right\rangle$.
2. Verify the virial theorem is satisfied for energy eigenstates.

Answer for Exercise 1.1

Part 1. Using

$$\begin{aligned}
x &= \frac{x_0}{\sqrt{2}} \left(a + a^\dagger \right) \\
p &= \frac{i \hbar}{x_0 \sqrt{2}} \left(a^\dagger - a \right) \\
a(t) &= a(0) e^{-i \omega t} \\
a(0) \left| n \right\rangle &= \sqrt{n} \left| n - 1 \right\rangle \\
a^\dagger(0) \left| n \right\rangle &= \sqrt{n + 1} \left| n + 1 \right\rangle \\
x_0^2 &= \frac{\hbar}{\omega m},
\end{aligned} \tag{1.1}$$

we have

$$\begin{aligned}
\left\langle m \right| x \left| n \right\rangle &= \frac{x_0}{\sqrt{2}} \left\langle m \right| \left(a + a^\dagger \right) \left| n \right\rangle \\
&= \frac{x_0}{\sqrt{2}} \left\langle m \right| \left(e^{-i \omega t} \sqrt{n} \left| n - 1 \right\rangle + e^{i \omega t} \sqrt{n + 1} \left| n + 1 \right\rangle \right) \\
&= \frac{x_0}{\sqrt{2}} \left(\delta_{m, n-1} e^{-i \omega t} \sqrt{n} + \delta_{m, n+1} e^{i \omega t} \sqrt{n + 1} \right),
\end{aligned} \tag{1.2}$$

$$
\begin{aligned}
\langle m| x^2 |n\rangle &= \frac{x_0^2}{2} \langle m| \left(a + a^\dagger\right)^2 |n\rangle \\
&= \frac{x_0^2}{2} \left(e^{i\omega t}\sqrt{m} \langle m-1| + e^{-i\omega t}\sqrt{m+1} \langle m+1|\right) \left(e^{-i\omega t}\sqrt{n} |n-1\rangle + e^{i\omega t}\sqrt{n+1} |n+1\rangle\right) \\
&= \frac{x_0^2}{2} \left(\delta_{m+1,n+1}\sqrt{(m+1)(n+1)}\right. \\
&\left. + \delta_{m+1,n-1}\sqrt{(m+1)n}e^{-2i\omega t} + \delta_{m-1,n+1}\sqrt{m(n+1)}e^{2i\omega t} + \delta_{m-1,n-1}\sqrt{mn}\right),
\end{aligned} \tag{1.3}
$$

$$
\begin{aligned}
\langle m| p |n\rangle &= \frac{i\hbar}{\sqrt{2}x_0} \langle m| \left(a^\dagger - a\right) |n\rangle \\
&= \frac{i\hbar}{\sqrt{2}x_0} \langle m| \left(e^{i\omega t}\sqrt{n+1} |n+1\rangle - e^{-i\omega t}\sqrt{n} |n-1\rangle\right) \\
&= \frac{i\hbar}{\sqrt{2}x_0} \left(\delta_{m,n+1}e^{i\omega t}\sqrt{n+1} - \delta_{m,n-1}e^{-i\omega t}\sqrt{n}\right),
\end{aligned} \tag{1.4}
$$

$$
\begin{aligned}
\langle m| p^2 |n\rangle &= \frac{\hbar^2}{2x_0^2} |m\rangle \left(a - a^\dagger\right) \left(a^\dagger - a\right) |n\rangle \\
&= \frac{\hbar^2}{2x_0^2} \left(-e^{-i\omega t}\sqrt{m+1} \langle m+1| + e^{i\omega t}\sqrt{m} \langle m-1|\right) \left(e^{i\omega t}\sqrt{n+1} |n+1\rangle - e^{-i\omega t}\sqrt{n} |n-1\rangle\right) \\
&= \frac{\hbar^2}{2x_0^2} \left(\delta_{m+1,n+1}\sqrt{(m+1)(n+1)}\right. \\
&\left. + \delta_{m+1,n-1}\sqrt{(m+1)n}e^{-2i\omega t} + \delta_{m-1,n+1}\sqrt{m(n+1)}e^{2i\omega t} + \delta_{m-1,n-1}\sqrt{mn}\right).
\end{aligned} \tag{1.5}
$$

For the anticommutator $\{x, p\}$, we have

$$
\begin{aligned}
\{x, p\} &= \frac{i\hbar}{2} \left(\left(ae^{-i\omega t} + a^\dagger e^{i\omega t}\right) \left(a^\dagger e^{i\omega t} - ae^{-i\omega t}\right) - \left(a^\dagger e^{i\omega t} - ae^{-i\omega t}\right) \left(ae^{-i\omega t} + a^\dagger e^{i\omega t}\right)\right) \\
&= \frac{i\hbar}{2} \left(-a^2e^{-2i\omega t} + (a^\dagger)^2e^{2i\omega t} + aa^\dagger - a^\dagger a + a^2e^{-2i\omega t} - (a^\dagger)^2e^{2i\omega t} - a^\dagger a + aa^\dagger\right) \\
&= i\hbar \left(aa^\dagger - a^\dagger a\right),
\end{aligned} \tag{1.6}
$$

so

$$
\begin{aligned}
\langle m| \{x, p\} |n\rangle &= i\hbar \langle m| \left(aa^\dagger - a^\dagger a\right) |n\rangle \\
&= i\hbar \langle m| \left(\sqrt{(n+1)^2} |n\rangle - \sqrt{n^2} |n\rangle\right) \\
&= i\hbar \langle m| (2n+1) |n\rangle .
\end{aligned} \tag{1.7}
$$

Part 2. For the SHO, the virial theorem requires $\langle p^2/m \rangle = \langle m\omega x^2 \rangle$. That momentum expectation with respect to the eigenstate $|n\rangle$ is

$$\langle p^2/m \rangle = \frac{\hbar^2}{2x_0^2 m} \left(\sqrt{(n+1)(n+1)} + \sqrt{nn} \right) = \frac{\hbar^2 m\omega}{2\hbar m} (2n+1) = \hbar\omega \left(n + \frac{1}{2} \right). \tag{1.8}$$

For the position expectation we've got

$$\begin{aligned} \langle m\omega x^2 \rangle &= \frac{m\omega^2 x_0^2}{2} \left(\sqrt{(n+1)(n+1)} + \sqrt{nn} \right) \\ &= \frac{m\omega^2 \hbar}{2m\omega} \left(\sqrt{(n+1)(n+1)} + \sqrt{nn} \right) \\ &= \frac{\omega\hbar}{2} (2n+1) \\ &= \omega\hbar \left(n + \frac{1}{2} \right). \end{aligned} \tag{1.9}$$

This shows that the virial theorem holds for the SHO Hamiltonian for eigenstates.

Bibliography

[1] Jun John Sakurai and Jim J Napolitano. *Modern quantum mechanics*. Pearson Higher Ed, 2014. 1.1