Problem 2.11

(a) Compute $\langle x\rangle$, $\langle p\rangle$, $\langle x^2\rangle$, and $\langle p^2\rangle$, for the states ψ_0 (Equation 2.60) and ψ_1 (Equation 2.63), by explicit integration. *Comment:* In this and other problems involving the harmonic oscillator it simplifies matters if you introduce the variable $\xi \equiv \sqrt{m\omega/\hbar}x$ and the constant $\alpha \equiv (m\omega/\pi\hbar)^{1/4}$.

(b) Check the uncertainty principle for these states.

(c) Compute $\langle T\rangle$ and $\langle V\rangle$ for these states. (No new integration allowed!) Is their sum what you would expect?

Solution

In Problem 2.10 the first three eigenstates of the harmonic oscillator were found to be

$$\begin{aligned}
\psi_0(x) &= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega}{2\hbar}x^2\right)\\
\psi_1(x) &= \left(\frac{4m^3\omega^3}{\pi\hbar^3}\right)^{1/4}x\exp\left(-\frac{m\omega}{2\hbar}x^2\right)\\
\psi_2(x) &= \left(\frac{m\omega}{4\pi\hbar}\right)^{1/4}\left(\frac{2m\omega}{\hbar}x^2-1\right)\exp\left(-\frac{m\omega}{2\hbar}x^2\right).
\end{aligned}$$

Note that some of the following integrals are zero because the integral is of an odd function over a symmetric interval. Use the formulas inside the back cover to evaluate the others.

Eigenstate ψ_0

Calculate the expectation value of x.

$$\begin{aligned}
\langle x\rangle &= \int_{-\infty}^{\infty}\psi_0^*(x)(x)\psi_0(x)\,dx\\
&= \int_{-\infty}^{\infty}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega}{2\hbar}x^2\right)(x)\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega}{2\hbar}x^2\right)dx\\
&= \sqrt{\frac{m\omega}{\pi\hbar}}\int_{-\infty}^{\infty}x\exp\left(-\frac{m\omega}{\hbar}x^2\right)dx\\
&= 0
\end{aligned}$$

Calculate the expectation value of x^2.

$$\begin{aligned}
\langle x^2\rangle &= \int_{-\infty}^{\infty}\psi_0^*(x)(x^2)\psi_0(x)\,dx\\
&= \int_{-\infty}^{\infty}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega}{2\hbar}x^2\right)(x^2)\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega}{2\hbar}x^2\right)dx\\
&= \sqrt{\frac{m\omega}{\pi\hbar}}\int_{-\infty}^{\infty}x^2\exp\left(-\frac{m\omega}{\hbar}x^2\right)dx\\
&= 2\sqrt{\frac{m\omega}{\pi\hbar}}\int_0^{\infty}x^2\exp\left[-\frac{x^2}{\left(\sqrt{\frac{\hbar}{m\omega}}\right)^2}\right]dx = 2\sqrt{\frac{m\omega}{\pi\hbar}}\cdot\sqrt{\pi}\,\frac{2!}{1!}\left(\frac{\sqrt{\frac{\hbar}{m\omega}}}{2}\right)^3 = \frac{\hbar}{2m\omega}
\end{aligned}$$

Calculate the expectation value of p.

$$\begin{aligned}
\langle p\rangle &= \int_{-\infty}^{\infty} \psi_0^*(x)\left(-i\hbar\frac{\partial}{\partial x}\right)\psi_0(x)\,dx \\
&= -i\hbar\int_{-\infty}^{\infty}\psi_0^*(x)\frac{d\psi_0}{dx}\,dx \\
&= -i\hbar\int_{-\infty}^{\infty}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega}{2\hbar}x^2\right)\frac{d}{dx}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega}{2\hbar}x^2\right)dx \\
&= -i\hbar\int_{-\infty}^{\infty}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega}{2\hbar}x^2\right)\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega}{2\hbar}x^2\right)\left(-\frac{m\omega}{\hbar}x\right)dx \\
&= im\omega\sqrt{\frac{m\omega}{\pi\hbar}}\int_{-\infty}^{\infty}x\exp\left(-\frac{m\omega}{\hbar}x^2\right)dx \\
&= 0
\end{aligned}$$

Calculate the expectation value of p^2.

$$\begin{aligned}
\langle p^2\rangle &= \int_{-\infty}^{\infty}\psi_0^*(x)\left(-i\hbar\frac{\partial}{\partial x}\right)^2\psi_0(x)\,dx \\
&= \int_{-\infty}^{\infty}\psi_0^*(x)\left(-\hbar^2\frac{\partial^2}{\partial x^2}\right)\psi_0(x)\,dx \\
&= -\hbar^2\int_{-\infty}^{\infty}\psi_0^*(x)\frac{d^2\psi_0}{dx^2}\,dx \\
&= -\hbar^2\int_{-\infty}^{\infty}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega}{2\hbar}x^2\right)\frac{d^2}{dx^2}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega}{2\hbar}x^2\right)dx \\
&= -\hbar^2\int_{-\infty}^{\infty}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega}{2\hbar}x^2\right)\frac{d}{dx}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega}{2\hbar}x^2\right)\left(-\frac{m\omega}{\hbar}x\right)dx \\
&= -\hbar^2\int_{-\infty}^{\infty}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega}{2\hbar}x^2\right)\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\left[\exp\left(-\frac{m\omega}{2\hbar}x^2\right)\left(-\frac{m\omega}{\hbar}x\right)^2+\exp\left(-\frac{m\omega}{2\hbar}x^2\right)\left(-\frac{m\omega}{\hbar}\right)\right]dx \\
&= -\hbar^2\sqrt{\frac{m\omega}{\pi\hbar}}\int_{-\infty}^{\infty}\left[\left(-\frac{m\omega}{\hbar}x\right)^2+\left(-\frac{m\omega}{\hbar}\right)\right]\exp\left(-\frac{m\omega}{\hbar}x^2\right)dx \\
&= -\hbar^2\sqrt{\frac{m^3\omega^3}{\pi\hbar^3}}\int_{-\infty}^{\infty}\left(\frac{m\omega}{\hbar}x^2-1\right)\exp\left(-\frac{m\omega}{\hbar}x^2\right)dx
\end{aligned}$$

Make the following substitution.

$$\begin{aligned}
\xi &= \sqrt{\frac{m\omega}{\hbar}}x \\
d\xi &= \sqrt{\frac{m\omega}{\hbar}}\,dx \quad\rightarrow\quad dx = \sqrt{\frac{\hbar}{m\omega}}\,d\xi
\end{aligned}$$

Consequently,

$$\begin{aligned}
\langle p^2 \rangle &= -\hbar^2 \sqrt{\frac{m^3\omega^3}{\pi\hbar^3}} \int_{-\infty}^{\infty} (\xi^2 - 1)e^{-\xi^2} \left(\sqrt{\frac{\hbar}{m\omega}}\, d\xi \right) \\
&= -\frac{\hbar m\omega}{\sqrt{\pi}} \int_{-\infty}^{\infty} (\xi^2 - 1)e^{-\xi^2}\, d\xi \\
&= -\frac{2\hbar m\omega}{\sqrt{\pi}} \int_{0}^{\infty} (\xi^2 - 1)e^{-\xi^2}\, d\xi \\
&= -\frac{2\hbar m\omega}{\sqrt{\pi}} \left(\int_0^{\infty} \xi^2 e^{-\xi^2}\, d\xi - \int_0^{\infty} e^{-\xi^2}\, d\xi \right) \\
&= -\frac{2\hbar m\omega}{\sqrt{\pi}} \left[\sqrt{\pi}\, \frac{2!}{1!} \left(\frac{1}{2}\right)^3 - \sqrt{\pi} \left(\frac{1}{2}\right) \right] \\
&= -\frac{2\hbar m\omega}{\sqrt{\pi}} \left(-\frac{\sqrt{\pi}}{4} \right) \\
&= \frac{\hbar m\omega}{2}.
\end{aligned}$$

The standard deviation in x is

$$\sigma_x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sqrt{\frac{\hbar}{2m\omega}},$$

and the standard deviation in p is

$$\sigma_p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \sqrt{\frac{\hbar m\omega}{2}}.$$

Taking the product of these two,

$$\sigma_x \sigma_p = \sqrt{\frac{\hbar}{2m\omega}} \sqrt{\frac{\hbar m\omega}{2}} = \frac{\hbar}{2},$$

we see that Heisenberg's uncertainty principle ($\sigma_x\sigma_p \geq \hbar/2$) is satisfied for the ground state. The expectations of potential energy and kinetic energy are respectively

$$\begin{aligned}
\langle V \rangle &= \left\langle \frac{1}{2} m\omega^2 x^2 \right\rangle = \frac{1}{2} m\omega^2 \langle x^2 \rangle = \frac{1}{2} m\omega^2 \left(\frac{\hbar}{2m\omega} \right) = \frac{\hbar\omega}{4} \\
\langle T \rangle &= \left\langle \frac{p^2}{2m} \right\rangle = \frac{1}{2m} \langle p^2 \rangle = \frac{1}{2m} \left(\frac{\hbar m\omega}{2} \right) = \frac{\hbar\omega}{4}.
\end{aligned}$$

Adding them together gives

$$\langle V \rangle + \langle T \rangle = \frac{\hbar\omega}{2},$$

which is the energy of the ground state.

Eigenstate ψ_1

Calculate the expectation value of x.

$$\begin{aligned}
\langle x\rangle &= \int_{-\infty}^{\infty} \psi_1^*(x)(x)\psi_1(x)\,dx \\
&= \int_{-\infty}^{\infty} \left(\frac{4m^3\omega^3}{\pi\hbar^3}\right)^{1/4} x\exp\left(-\frac{m\omega}{2\hbar}x^2\right)(x)\left(\frac{4m^3\omega^3}{\pi\hbar^3}\right)^{1/4} x\exp\left(-\frac{m\omega}{2\hbar}x^2\right)dx \\
&= \sqrt{\frac{4m^3\omega^3}{\pi\hbar^3}}\int_{-\infty}^{\infty} x^3\exp\left(-\frac{m\omega}{\hbar}x^2\right)dx \\
&= 0
\end{aligned}$$

Calculate the expectation value of x^2.

$$\begin{aligned}
\langle x^2\rangle &= \int_{-\infty}^{\infty} \psi_1^*(x)(x^2)\psi_1(x)\,dx \\
&= \int_{-\infty}^{\infty} \left(\frac{4m^3\omega^3}{\pi\hbar^3}\right)^{1/4} x\exp\left(-\frac{m\omega}{2\hbar}x^2\right)(x^2)\left(\frac{4m^3\omega^3}{\pi\hbar^3}\right)^{1/4} x\exp\left(-\frac{m\omega}{2\hbar}x^2\right)dx \\
&= \sqrt{\frac{4m^3\omega^3}{\pi\hbar^3}}\int_{-\infty}^{\infty} x^4\exp\left(-\frac{m\omega}{\hbar}x^2\right)dx \\
&= \sqrt{\frac{4\hbar}{\pi m\omega}}\int_{-\infty}^{\infty} \frac{m^2\omega^2}{\hbar^2}x^4\exp\left(-\frac{m\omega}{\hbar}x^2\right)dx
\end{aligned}$$

Make the following substitution.

$$\begin{aligned}
\xi &= \sqrt{\frac{m\omega}{\hbar}}x & &\rightarrow & \xi^4 &= \frac{m^2\omega^2}{\hbar^2}x^4 \\
d\xi &= \sqrt{\frac{m\omega}{\hbar}}\,dx & &\rightarrow & dx &= \sqrt{\frac{\hbar}{m\omega}}\,d\xi
\end{aligned}$$

Consequently,

$$\begin{aligned}
\langle x^2\rangle &= \sqrt{\frac{4\hbar}{\pi m\omega}}\int_{-\infty}^{\infty} \xi^4 e^{-\xi^2}\left(\sqrt{\frac{\hbar}{m\omega}}\,d\xi\right) \\
&= \frac{2}{\sqrt{\pi}}\frac{\hbar}{m\omega}\int_{-\infty}^{\infty} \xi^4 e^{-\xi^2}\,d\xi \\
&= \frac{4}{\sqrt{\pi}}\frac{\hbar}{m\omega}\int_{0}^{\infty} \xi^4 e^{-\xi^2}\,d\xi \\
&= \frac{4}{\sqrt{\pi}}\frac{\hbar}{m\omega}\cdot\sqrt{\pi}\,\frac{4!}{2!}\left(\frac{1}{2}\right)^5 \\
&= \frac{3\hbar}{2m\omega}.
\end{aligned}$$

Calculate the expectation value of p.

$$\begin{aligned}
\langle p\rangle &= \int_{-\infty}^{\infty} \psi_1^*(x)\left(-i\hbar\frac{\partial}{\partial x}\right)\psi_1(x)\,dx \\
&= -i\hbar\int_{-\infty}^{\infty} \psi_1^*(x)\frac{d\psi_1}{dx}\,dx \\
&= -i\hbar\int_{-\infty}^{\infty} \left(\frac{4m^3\omega^3}{\pi\hbar^3}\right)^{1/4} x\exp\left(-\frac{m\omega}{2\hbar}x^2\right)\frac{d}{dx}\left[\left(\frac{4m^3\omega^3}{\pi\hbar^3}\right)^{1/4} x\exp\left(-\frac{m\omega}{2\hbar}x^2\right)\right]dx \\
&= -i\hbar\int_{-\infty}^{\infty} \left(\frac{4m^3\omega^3}{\pi\hbar^3}\right)^{1/4} x\exp\left(-\frac{m\omega}{2\hbar}x^2\right)\left(\frac{4m^3\omega^3}{\pi\hbar^3}\right)^{1/4}\left[\exp\left(-\frac{m\omega}{2\hbar}x^2\right)+x\exp\left(-\frac{m\omega}{2\hbar}x^2\right)\left(-\frac{m\omega}{\hbar}x\right)\right]dx \\
&= -i\hbar\sqrt{\frac{4m^3\omega^3}{\pi\hbar^3}}\int_{-\infty}^{\infty} x\left(1-\frac{m\omega}{\hbar}x^2\right)\exp\left(-\frac{m\omega}{\hbar}x^2\right)dx \\
&= 0
\end{aligned}$$

Calculate the expectation value of p^2.

$$\begin{aligned}
\langle p^2\rangle &= \int_{-\infty}^{\infty} \psi_1^*(x)\left(-i\hbar\frac{\partial}{\partial x}\right)^2\psi_1(x)\,dx \\
&= \int_{-\infty}^{\infty} \psi_1^*(x)\left(-\hbar^2\frac{\partial^2}{\partial x^2}\right)\psi_1(x)\,dx \\
&= -\hbar^2\int_{-\infty}^{\infty} \psi_1^*(x)\frac{d^2\psi_1}{dx^2}\,dx \\
&= -\hbar^2\int_{-\infty}^{\infty} \left(\frac{4m^3\omega^3}{\pi\hbar^3}\right)^{1/4} x\exp\left(-\frac{m\omega}{2\hbar}x^2\right)\frac{d^2}{dx^2}\left[\left(\frac{4m^3\omega^3}{\pi\hbar^3}\right)^{1/4} x\exp\left(-\frac{m\omega}{2\hbar}x^2\right)\right]dx \\
&= -\hbar^2\int_{-\infty}^{\infty} \left(\frac{4m^3\omega^3}{\pi\hbar^3}\right)^{1/4} x\exp\left(-\frac{m\omega}{2\hbar}x^2\right)\left(\frac{4m^3\omega^3}{\pi\hbar^3}\right)^{1/4}\frac{d}{dx}\left[\exp\left(-\frac{m\omega}{2\hbar}x^2\right)+x\exp\left(-\frac{m\omega}{2\hbar}x^2\right)\left(-\frac{m\omega}{\hbar}x\right)\right]dx \\
&= -\hbar^2\int_{-\infty}^{\infty} \left(\frac{4m^3\omega^3}{\pi\hbar^3}\right)^{1/4} x\exp\left(-\frac{m\omega}{2\hbar}x^2\right)\left(\frac{4m^3\omega^3}{\pi\hbar^3}\right)^{1/4}\frac{d}{dx}\left[\left(1-\frac{m\omega}{\hbar}x^2\right)\exp\left(-\frac{m\omega}{2\hbar}x^2\right)\right]dx \\
&= -\hbar^2\sqrt{\frac{4m^3\omega^3}{\pi\hbar^3}}\int_{-\infty}^{\infty} x\exp\left(-\frac{m\omega}{2\hbar}x^2\right)\left[\left(-\frac{2m\omega}{\hbar}x\right)+\left(1-\frac{m\omega}{\hbar}x^2\right)\left(-\frac{m\omega}{\hbar}x\right)\right]\exp\left(-\frac{m\omega}{2\hbar}x^2\right)dx \\
&= -\hbar^2\sqrt{\frac{4m^3\omega^3}{\pi\hbar^3}}\int_{-\infty}^{\infty} x\left(-\frac{m\omega}{\hbar}x\right)\left[2+\left(1-\frac{m\omega}{\hbar}x^2\right)\right]\exp\left(-\frac{m\omega}{\hbar}x^2\right)dx \\
&= \hbar^2\sqrt{\frac{4m^3\omega^3}{\pi\hbar^3}}\int_{-\infty}^{\infty} \frac{m\omega}{\hbar}x^2\left(3-\frac{m\omega}{\hbar}x^2\right)\exp\left(-\frac{m\omega}{\hbar}x^2\right)dx
\end{aligned}$$

Make the following substitution.

$$\begin{aligned}
\xi &= \sqrt{\frac{m\omega}{\hbar}}x &\quad\rightarrow\quad \xi^2 &= \frac{m\omega}{\hbar}x^2 \\
d\xi &= \sqrt{\frac{m\omega}{\hbar}}\,dx &\quad\rightarrow\quad dx &= \sqrt{\frac{\hbar}{m\omega}}\,d\xi
\end{aligned}$$

As a result,

$$\begin{aligned}
\langle p^2 \rangle &= \hbar^2 \sqrt{\frac{4m^3\omega^3}{\pi\hbar^3}} \int_{-\infty}^{\infty} \xi^2(3-\xi^2)e^{-\xi^2} \left(\sqrt{\frac{\hbar}{m\omega}}\, d\xi \right) \\
&= \frac{2\hbar m\omega}{\sqrt{\pi}} \int_{-\infty}^{\infty} \xi^2(3-\xi^2)e^{-\xi^2}\, d\xi \\
&= \frac{4\hbar m\omega}{\sqrt{\pi}} \int_{0}^{\infty} \xi^2(3-\xi^2)e^{-\xi^2}\, d\xi \\
&= \frac{4\hbar m\omega}{\sqrt{\pi}} \left(3\int_0^\infty \xi^2 e^{-\xi^2}\, d\xi - \int_0^\infty \xi^4 e^{-\xi^2}\, d\xi \right) \\
&= \frac{4\hbar m\omega}{\sqrt{\pi}} \left[3 \cdot \sqrt{\pi}\, \frac{2!}{1!} \left(\frac{1}{2}\right)^3 - \sqrt{\pi}\, \frac{4!}{2!} \left(\frac{1}{2}\right)^5 \right] \\
&= \frac{4\hbar m\omega}{\sqrt{\pi}} \left(\frac{3\sqrt{\pi}}{8} \right) \\
&= \frac{3\hbar m\omega}{2}
\end{aligned}$$

The standard deviation in x is

$$\sigma_x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sqrt{\frac{3\hbar}{2m\omega}},$$

and the standard deviation in p is

$$\sigma_p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \sqrt{\frac{3\hbar m\omega}{2}}.$$

Taking the product of these two,

$$\sigma_x \sigma_p = \sqrt{\frac{3\hbar}{2m\omega}} \sqrt{\frac{3\hbar m\omega}{2}} = \frac{3\hbar}{2},$$

we see that Heisenberg's uncertainty principle ($\sigma_x\sigma_p \geq \hbar/2$) is satisfied for the first excited state. The expectations of potential energy and kinetic energy are respectively

$$\begin{aligned}
\langle V \rangle &= \left\langle \frac{1}{2} m\omega^2 x^2 \right\rangle = \frac{1}{2} m\omega^2 \langle x^2 \rangle = \frac{1}{2} m\omega^2 \left(\frac{3\hbar}{2m\omega} \right) = \frac{3\hbar\omega}{4} \\
\langle T \rangle &= \left\langle \frac{p^2}{2m} \right\rangle = \frac{1}{2m} \langle p^2 \rangle = \frac{1}{2m} \left(\frac{3\hbar m\omega}{2} \right) = \frac{3\hbar\omega}{4}.
\end{aligned}$$

Adding them together gives

$$\langle V \rangle + \langle T \rangle = \frac{3\hbar\omega}{2},$$

which is the energy of the first excited state.