Problem 3.37

Virial theorem. Use Equation 3.73 to show that

$$\frac{d}{dt}\langle xp\rangle = 2\langle T\rangle - \left\langle x\frac{\partial V}{\partial x}\right\rangle, \tag{3.112}$$

where T is the kinetic energy ($H = T + V$). In a *stationary* state the left side is zero (why?) so

$$2\langle T\rangle = \left\langle x\frac{dV}{dx}\right\rangle. \tag{3.113}$$

This is called the **virial theorem**. Use it to prove that $\langle T\rangle = \langle V\rangle$ for stationary states of the harmonic oscillator, and check that this is consistent with the results you got in Problems 2.11 and 2.12.

Solution

Start by expanding the left side with Equation 3.73.

$$\begin{aligned}
\frac{d}{dt}\langle xp\rangle &= \frac{i}{\hbar}\left\langle\left[\hat{H},\hat{x}\hat{p}\right]\right\rangle + \left\langle\frac{\partial}{\partial t}(xp)\right\rangle \\
&= \frac{i}{\hbar}\left\langle\Psi\left|\left[\hat{H},\hat{x}\hat{p}\right]\right|\Psi\right\rangle + \left\langle\Psi\left|\frac{\partial}{\partial t}(xp)\right|\Psi\right\rangle \\
&= \frac{i}{\hbar}\int_{-\infty}^{\infty}\Psi^*(x,t)\left[\hat{H},\hat{x}\hat{p}\right]\Psi(x,t)\,dx + \int_{-\infty}^{\infty}\Psi^*(x,t)\frac{\partial}{\partial t}(xp)\Psi(x,t)\,dx \\
&= \frac{i}{\hbar}\int_{-\infty}^{\infty}\Psi^*(x,t)\left(\hat{H}\hat{x}\hat{p} - \hat{x}\hat{p}\hat{H}\right)\Psi(x,t)\,dx + \int_{-\infty}^{\infty}\Psi^*(x,t)(0)\Psi(x,t)\,dx \\
&= \frac{i}{\hbar}\int_{-\infty}^{\infty}\Psi^*(x,t)\left[\left(\frac{\hat{p}^2}{2m} + V(x,t)\right)\hat{x}\hat{p} - \hat{x}\hat{p}\left(\frac{\hat{p}^2}{2m} + V(x,t)\right)\right]\Psi(x,t)\,dx \\
&= \frac{i}{\hbar}\int_{-\infty}^{\infty}\Psi^*(x,t)\left\{\left[\frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial x}\right)^2 + V(x,t)\right]x\left(-i\hbar\frac{\partial}{\partial x}\right)\right. \\
&\qquad\qquad \left. - x\left(-i\hbar\frac{\partial}{\partial x}\right)\left[\frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial x}\right)^2 + V(x,t)\right]\right\}\Psi(x,t)\,dx \\
&= \int_{-\infty}^{\infty}\Psi^*(x,t)\left\{\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)\right]x\frac{\partial}{\partial x}\right. \\
&\qquad\qquad \left. - x\frac{\partial}{\partial x}\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)\right]\right\}\Psi(x,t)\,dx \\
&= \int_{-\infty}^{\infty}\Psi^*(x,t)\left\{\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)\right]x\frac{\partial\Psi}{\partial x} - x\frac{\partial}{\partial x}\left[-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x,t)\Psi(x,t)\right]\right\}dx \\
&= \int_{-\infty}^{\infty}\Psi^*(x,t)\left\{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\left(x\frac{\partial\Psi}{\partial x}\right) + V(x,t)x\frac{\partial\Psi}{\partial x} + \frac{\hbar^2}{2m}x\frac{\partial^3\Psi}{\partial x^3} - x\frac{\partial}{\partial x}[V(x,t)\Psi(x,t)]\right\}dx
\end{aligned}$$

Evaluate the derivatives and simplify the result.

$$\begin{aligned}
\frac{d}{dt}\langle xp\rangle &= \int_{-\infty}^{\infty} \Psi^*(x,t)\left\{-\frac{\hbar^2}{2m}\frac{\partial}{\partial x}\left(\frac{\partial\Psi}{\partial x}+x\frac{\partial^2\Psi}{\partial x^2}\right)+V(x,t)x\frac{\partial\Psi}{\partial x}+\frac{\hbar^2}{2m}x\frac{\partial^3\Psi}{\partial x^3}-x\left[\frac{\partial V}{\partial x}\Psi(x,t)+V(x,t)\frac{\partial\Psi}{\partial x}\right]\right\}dx \\
&= \int_{-\infty}^{\infty} \Psi^*(x,t)\left[-\frac{\hbar^2}{2m}\left(2\frac{\partial^2\Psi}{\partial x^2}+\cancel{x\frac{\partial^3\Psi}{\partial x^3}}\right)+\cancel{xV(x,t)\frac{\partial\Psi}{\partial x}}+\cancel{\frac{\hbar^2}{2m}x\frac{\partial^3\Psi}{\partial x^3}}-x\frac{\partial V}{\partial x}\Psi(x,t)-\cancel{xV(x,t)\frac{\partial\Psi}{\partial x}}\right]dx \\
&= \int_{-\infty}^{\infty} \Psi^*(x,t)\left[2\left(-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}\right)-x\frac{\partial V}{\partial x}\Psi(x,t)\right]dx \\
&= \int_{-\infty}^{\infty} \Psi^*(x,t)\left[2\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)-x\frac{\partial V}{\partial x}\right]\Psi(x,t)\,dx \\
&= \int_{-\infty}^{\infty} \Psi^*(x,t)\left[2\left(\frac{\hat{p}^2}{2m}\right)-\hat{x}\frac{\partial V}{\partial x}\right]\Psi(x,t)\,dx \\
&= 2\int_{-\infty}^{\infty} \Psi^*(x,t)\left(\frac{\hat{p}^2}{2m}\right)\Psi(x,t)\,dx-\int_{-\infty}^{\infty} \Psi^*(x,t)\left(\hat{x}\frac{\partial V}{\partial x}\right)\Psi(x,t)\,dx \\
&= 2\left\langle \Psi \,\middle|\, \frac{\hat{p}^2}{2m} \,\middle|\, \Psi\right\rangle - \left\langle \Psi \,\middle|\, \hat{x}\frac{\partial V}{\partial x} \,\middle|\, \Psi\right\rangle \\
&= 2\left\langle \frac{p^2}{2m}\right\rangle - \left\langle x\frac{\partial V}{\partial x}\right\rangle
\end{aligned}$$

Therefore, letting T represent the kinetic energy,

$$\boxed{\frac{d}{dt}\langle xp\rangle = 2\langle T\rangle - \left\langle x\frac{\partial V}{\partial x}\right\rangle.}$$

The position-space wave function for a stationary state is of the form,

$$\Psi_n(x,t)=\psi_n(x)e^{-iE_nt/\hbar},$$

so the boxed equation becomes

$$\begin{aligned}
2\langle T\rangle - \left\langle x\frac{\partial V}{\partial x}\right\rangle &= \frac{d}{dt}\langle xp\rangle \\
&= \frac{d}{dt}\langle \Psi_n \,|\, \hat{x}\hat{p} \,|\, \Psi_n\rangle \\
&= \frac{d}{dt}\int_{-\infty}^{\infty} \Psi_n^*(x,t)(\hat{x}\hat{p})\Psi_n(x,t)\,dx \\
&= \frac{d}{dt}\int_{-\infty}^{\infty} \left[\psi_n^*(x)e^{iE_nt/\hbar}\right]x\left(-i\hbar\frac{\partial}{\partial x}\right)\left[\psi_n(x)e^{-iE_nt/\hbar}\right]dx \\
&= -i\hbar\frac{d}{dt}\int_{-\infty}^{\infty} \psi^*(x)e^{iE_nt/\hbar}x\frac{d\psi_n}{dx}e^{-iE_nt/\hbar}\,dx \\
&= -i\hbar\frac{d}{dt}\int_{-\infty}^{\infty} \psi^*(x)x\frac{d\psi_n}{dx}\,dx = -i\hbar\int_{-\infty}^{\infty}\frac{\partial}{\partial t}\left[\psi^*(x)x\frac{d\psi_n}{dx}\right]dx = -i\hbar\int_{-\infty}^{\infty}(0)\,dx = 0.
\end{aligned}$$

Therefore, for a stationary state,

$$\boxed{2\langle T\rangle = \left\langle x\frac{\partial V}{\partial x}\right\rangle.}$$

In the case of a harmonic oscillator potential, $V = (1/2)m\omega^2x^2$, this equation becomes

$$\begin{aligned}2\langle T\rangle &= \left\langle x\frac{dV}{dx}\right\rangle \\ &= \left\langle x\frac{d}{dx}\left(\frac{1}{2}m\omega^2x^2\right)\right\rangle \\ &= \langle x\left(m\omega^2x\right)\rangle \\ &= 2\left\langle \frac{1}{2}m\omega^2x^2\right\rangle \\ &= 2\langle V\rangle,\end{aligned}$$

that is,

$$\langle T\rangle = \langle V\rangle.$$

What has to be checked in Problems 2.11 and 2.12, then, is that

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

In Problem 2.11,

$$\begin{aligned}&\text{Zeroth Eigenstate:} \quad \langle x^2\rangle = \frac{\hbar}{2m\omega} \qquad \text{and} \qquad \langle p^2\rangle = \frac{\hbar m\omega}{2} \\ &\text{First Eigenstate:} \quad \langle x^2\rangle = \frac{3\hbar}{2m\omega} \qquad \text{and} \qquad \langle p^2\rangle = \frac{3\hbar m\omega}{2},\end{aligned}$$

so equation (1) is satisfied for the first two stationary states. In Problem 2.12,

$$n\text{th Eigenstate:} \quad \langle x^2\rangle = \frac{\hbar}{2m\omega}(2n+1) \qquad \text{and} \qquad \langle p^2\rangle = \frac{\hbar m\omega}{2}(2n+1),$$

so equation (1) is satisfied for the nth stationary state as well.